Serge Marguet

# The Physics of Nuclear Reactors 

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To my parents Josette and Daniel who supported my studies.
To my wife Agnès who continues to support me...!
To my children Hélène and Vincent, who excite my immune system!

## Foreword to the 2011 Edition

In the context of a worldwide economic crisis, what better indication could there be than the publication of this textbook on reactor physics?

Renunciation of the policy of adding further capacity to electrical production facilities in Europe, the immense energy requirements of countries such as China, India, and Brazil, and the growing international awareness that energy is a rare and expensive commodity are so many factors militating in favor of the proper use of the means of electricity production.

Furthermore, the avowed official desire to combat climate change and reduce energy costs means that renewable energy and nuclear production are priorities. Nuclear energy is once again making vigorous strides forwards, as attested in France in particular by the commissioning of the EPR in 2012, 80 years after discovery of the neutron by James Chadwick in 1932. The brief history of civil nuclear power shows that it is not possible to harness this energy in the long run without flawless safety levels, in all places and at all times.

Experts distinguish three safety functions: confinement of radioactive products, reliable removal of decay heat, and complete control over reactivity. To ensure that these conditions are met, the branches of neutron physics, fluid mechanics, thermal physics, materials physics, and chemistry have an essential role to play. Neutron physics is the science that describes and explains the behavior of neutrons in matter and the reactions they induce. In order to guarantee complete control of reactivity, a solid knowledge of neutron physics is indispensable in order to be able to define the proper measures to be taken, beginning with the reactor design stage and then throughout decades of operation.

Achieving complete understanding of the complex physical phenomena that occur in a nuclear installation and displayed to the operation engineers via monitors and computers in the control rooms is of cardinal importance for the optimal operation of power reactors (440 in service in 2009, a number that will doubtless rise two- or threefold by 2030 or 2040), of experimental reactors for deepening our level of understanding, and of laboratories and facilities for fuel cycle studies that are set to increase worldwide.

This textbook addresses all aspects of neutron physics: experts, engineers, and students will find between its covers a host of scientific references that will enable them to acquire, maintain, and improve their skills.

It is my hope that it will be used by the large community of engineers working in the service of peaceful use of nuclear energy, a lasting energy form, for the greater good of mankind.


World Association of Nuclear Operators (WANO) Paris, France

## Foreword to the 2017 Edition

The supply of clean, affordable, and reliable energy is a global challenge. The projected increase in populations, particularly in Africa and Asia, means that by 2035 global energy needs are predicted to increase by $50 \%$ over 2015 levels. The increasing evidence of man-made climate change has given greater prominence for low carbon technologies such as renewables, nuclear, and carbon capture and storage which should be developed and deployed widely. The Paris Agreement on climate change (2016) has shown governments' resolve to reduce the world's greenhouse gas emissions by accelerating the deployment of such technologies.

Against this background, nuclear energy is a critically important part of the global energy mix. Today, nuclear power accounts for over $10 \%$ of the world's electricity generation; over 440 reactors are operating around the world, delivering clean electricity to the grid. In 2017, there are more reactors being built than at any time during the previous 25 years. Sixty reactors are currently under construction in fourteen countries, including more than one third of these in China and others in countries which are new to nuclear, such as the United Arab Emirates.

However in 2011, the Tōhoku earthquake and tsunami led to the nuclear accident at the Fukushima Daiichi plant which has, alongside previous nuclear accidents, emphasized the importance of nuclear safety and three crucial safety functions: confinement of radioactive products, reliable removal of decay heat, and complete control over reactivity.

To ensure that these functions are delivered effectively, the branches of neutron physics, fluid dynamics, reactor physics, materials science, mechanical engineering, and chemistry/corrosion each have an essential role to play. Each of these technical fields is important in its own right as are the synergies between them. However, peculiar to nuclear science and engineering is the understanding of neutrons in materials and the reactions they induce. In order to ensure the control of the reactivity in operating reactor cores, a full understanding of neutron physics is required. Achieving a full understanding of the complex physical mechanisms that occur in a nuclear power reactor ensures both good design and safe operations.

This textbook addresses all aspects of neutron physics creating a body of scientific knowledge and supporting references that will be invaluable to those learning about and responsible for nuclear reactor systems.

I commend this textbook to students, engineers, experts, and reactor operators as a means to learn and maintain an up-to-date knowledge of such an important field of nuclear science.


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Andrew H. Sherry
Chief Scientist of NLL

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This book would not have been possible without the friendly assistance of Paul Reuss: his advice was precious and his proofreading extremely scrupulous. If neutron physics is a kingdom, then Paul is undoubtedly one of its princes since his technical expertise is equaled only by his modesty, two areas that I should certainly work on personally! My first contact with Paul dates back to my very first day at EDF in a sense, namely September 1, 1987. My director had left two things for me on my empty desk: the output listing of the COCCINELLE code and the renowned neutron physics treatise by Jean Bussac and Paul Reuss, the bilious green 1985 edition that everyone in the department referred to simply as "Reuss", in spite of Bussac's co-authorship. On asking my colleagues about some physics question or other for the third time, I was told "It's in Reuss", and I realized that I might have to go through this thick textbook thoroughly. I do not feel that I wasted my time in so doing! Later on, I was lucky enough to attend Paul's lectures as part of the Reactor Physics Master's at Saclay. I always marveled at his crystal clear explanations.

I also wish to thank my colleague and reactor physics expert, Michel Lam-Hime, for giving up (an enormous amount of) his personal time to proofread this book. My thoughts also go out to a few colleagues and close friends: Philippe Tétart, Patrick Erhard, and David Couyras, who were the stoic guinea pigs on whom I tested my craziest ideas, sometimes very late in the evening. Their judicious comments and remarks resulted in numerous improvements. Finally, I would like to thank JeanMichel Delbecq as well, my ex-Head of Department and member of the editorial committee at EDF, who believed in this project from the outset, Laurent Stricker, who did me the honor of writing the foreword to the 2011 edition, and Professor Andrew Sherry for the foreword to this edition.

At least, I would like to thank Electricité de France for the funding of the English translation, especially Bertrand Bouriquet for his enthusiastic support to this project. It would be a shame to forget Ansar Calloo (EDF/R\&D), whose translation is far beyond my poor level in English and Patrick Saunders (Novatrad) for his very
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Finally, SPI-global (Saravanan and team!) made an amazing job increasing the global quality of this English version.

## Introduction

Reactor physics is a young branch of science. It is widely held to have been born on December 2, 1942, in Chicago, with the news that "the Italian navigator has just landed in the New World", a coded sentence informing all authorized persons that the Italian, Enrico Fermi, had succeeded in his prodigious feat of diverging a uranium and graphite pile. However, very soon after this incredible feat of which the general public was largely unaware, this young science struck terror into the world with the explosion of two US atomic bombs over the Japanese cities of Hiroshima and Nagasaki, on August 6 and 9, 1945. The Land of the Rising Sun was brought to its knees by nuclear fire. Humanity was led wincing into the atomic age, filled with a mixture of fear and fascination. Since then, public interest has never waned thanks to tireless efforts of popularization.

The atomic age ushered in by scientists held out hope of unlimited energy, possibly free (according to the publications of the time), and to the end of war. Subsequent events unfortunately showed this dream to be an unrealizable utopia. The short supply on Earth of fissile material is already of great concern, and as for warfare. . . clearly when one war stops, another breaks out elsewhere on the planet. Reactor physics flourished in the 1950s and 1960s. The construction of large power reactors in the 1970s and 1980s led to intensive development of this technology, yielding sustainable technologies such as reactors running on natural uranium cooled with carbon gas and moderated by graphite, and pressurized water reactors, which form the backbone of the French reactor fleet. At the same time, the underlying physics became more stable: nuclear data were increasingly abundant and filled large databases, and the notation specific to the field of neutron physics became established. The knowledge of physicists was sustained through large-scale calculation codes, while generations of numerical physicists improved these codes thanks to breakthroughs in ever more elaborate and complex numerical methods.


Popularization of the atomic age reached its peak in the 1950s (here we see a special edition of the French science magazine, "Science et Vie" [Science and Life] published in 1958, the Marguet collection, courtesy Science et Vie)

In 1979, the accident at the Three Mile Island 2 reactor in the USA shook the scientific community; the reactor core was totally destroyed, despite such an accident being deemed impossible on account of all the precautionary measures taken. As a result of the almost complete lack of release of radioactive matter into the environment, awareness among the general public of the inherent dangers of the accident did not peak, but it created massive unease among scientists. Murphy's Law had been confirmed once more. However, in 1986, the Chernobyl accident in Ukraine, in which most of the core was expelled into the environment, contaminating significant areas and with far-reaching effects throughout Europe, created a terrible shock.

Civil nuclear energy programs were now perceived in the public mind as a huge threat to humanity, and hostility towards the nuclear technocrats gathered pace. In France, the combined action of the media and of the ecological parties, coupled with public defiance, led to decommissioning of the SuperPhénix fast-neutron reactor. The nuclear age stooped from splendor to misery, as the question of disposal of long-lasting nuclear waste materials scared the public, and scientists toiled without success to find a viable alternative to deep burial.

By the end of the 1990s, as students showed disaffection with the so-called hard sciences, the popularity of nuclear engineering had sunk to a new low, with the

Master's in Reactor Physics almost being phased out in the mid-1990s owing to the lack of students and the poor prospects for renewal of the reactor fleet. However, in the 2000s, scientists showed beyond doubt that global warming was due to human activities and to the release of greenhouse gases into the atmosphere. Indeed, the oil crisis accompanying the wane of that particular fuel (total depletion within 40 years was being touted in 2008!) heralded a revival of the fortunes of nuclear energy; the latter does not produce greenhouse gases and it is assumed that the requisite natural resources will last ten times longer than oil, and plutonium could well prove to be the wildcard to replace uranium 235, which may run out before the advent of fusion.

After a period of dwindling in human resources and loss of expertise over the years (in 2008, the French situation in terms of expertise in fast neutron reactors which had to be set up from scratch after the retirement of the SuperPhénix generation, is characteristic, and even perhaps a caricature of this state of affairs), know-how regarding reactor physics lay buried in the extensive computational codes. For this reason, it seemed to me timely to write this textbook amid the resurgence of interest in nuclear engineering to ensure renewal of the international reactor fleet, along with increasing energy demand.

This textbook is thus addressed to students in higher studies, engineering students in nuclear energy and engineering, and engineers and research scientists at large who wish to review the founding notions of their professions. It is the culmination of 15 years of lectures given at the "Ecole Nationale Supérieure d'Ingénieurs" in Bourges (France), where I was able to observe (with great pleasure) the renewed interest of students in this particular field. I wanted this textbook to be both educational in terms of its content and convivial through its illustrations, and I hope that it will provide answers for beginners and knowledgeable readers alike. The textbook first sets out the minimum knowledge in nuclear physics required for an understanding of more advanced concepts. The subject itself has become a separate branch of science. It then examines neutron physics, which describes the intrinsic behavior of neutrons in matter, and then reactor physics, which is the art of making a pile critical in order to produce heat. The thermal hydraulics of the coolant material and the thermal physics of the nuclear fuel that are often associated with reactor physics will be explored in a separate textbook entitled "Physique des accidents dans les réacteurs nucléaires" [Physics of accidents in nuclear reactors]; these very important subject areas are too vast to be presented in the present volume. Indeed, as part of the generation that grew up with water reactors and because of my experience in this area, I have focused chiefly on Pressurized Water Reactors, which have flourished during my career at Électricité De France. Throughout the various chapters, I have done my utmost to review the history of this young science that is currently enjoying a revival.

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## Part I <br> Neutronics

## Chapter 1 <br> Fundamentals of Nuclear Physics

Reactor physics is a combination of nuclear physics and neutronics, both of which are essential for a comprehensive understanding of the phenomena involved. This chapter presents the rudiments of nuclear physics necessary for a reactor physicist.
(Fernandez 2006; Heisenberg 1953)

### 1.1 Chemical Elements

All of the everyday physical matter around us is made up of atoms (from the Greek atomos meaning "that which cannot be cut", "indivisible"), the characteristic particles present in all chemical elements. The chemical elements are defined by their chemical properties, which depend on the number of protons, $Z$, called the atomic number. In fact, the chemical properties of a given element depend on its electron structure, and thus on the number of electrons it contains. Since atoms are neutral, the number of electrons within the electron structure of a given atom is equal to the number of protons it contains. The elements are characterized by their symbol (denoted $X$ ). In 1868, the Russian chemist Dimitri Mendeleev formulated his famous periodic table of elements, which was predictive and continues to evolve even today. A chemical element is represented by a capital letter (e.g. iodine $=I$ ), or a capital letter followed by a small letter (e.g. copper $=C u$ ):
${ }_{92} U$ element $92=$ chemical element uranium with 92 protons
${ }_{2} \mathrm{He}$ element $2=$ chemical element helium with 2 protons
An element is said to be natural if it occurs naturally. It is said to be synthetic if it is man-made. Examples of natural elements are lead $(P b)$, sodium $(N a)$, potassium
$(K)$, uranium $(U)$ and tungsten $(W)$. Synthetic elements include plutonium ( Pu ), discovered in 1940 by a team led by Glenn Seaborg, ${ }^{1}$ neptunium ( $N p$ ), discovered in 1940 by McMillan and Abelson (Mathieu 1991, p. 234) as well as technetium ( $Z=43$ ) and promethium $(Z=61)$, which are lighter in mass than uranium. Using particle accelerators, element 118, or ununoctium, was synthesized in 1999, but its identification remains to be finalized since the last decay product in its radioactive chain is an unknown isotope! The latest elements to be discovered are generally named after a known physicist. IUPAC (International Union of Pure and Applied Chemistry) confers the official name on the new elements after dealing with the usual "squabbles" concerning precedence among the various laboratories applying for a name. Seaborgium, the name given to element 106 since 1994 in honor of Glenn Seaborg, discoverer of plutonium, was initially refused by IUPAC on the grounds that it was unusual to name an element after a living scientist, but in 1997, the IUPAC finally decided to accord this privilege to Seaborg, then aged 85. Other examples include rutherfordium (element 104, symbol $R f$ ) named in honor of Ernest Rutherford, who discovered the nucleus; bohrium (element 107, symbol $B h$ ), in honor of Niels Bohr; meitnerium (element 109, symbol $M t$ ) in honor of Lise Meitner, unjustly overlooked for a Nobel prize. It was the German Julius Lothar Meyer ${ }^{2}$ (1830-1895) and the Russian Dimitri Mendeleev (1834-1907) who, independently between 1868 and 1869, suggested a table for the classification of the chemical elements by weight and chemical properties. Mendeleev's table, or the Periodic Table of Elements, contained the 64 elements that were known at that time (Rosmorduc 1987, p. 257), arranged in lines and columns according to their mass and chemical properties (from lightest to heaviest). This table (Fig. 1.1) was predictive, and certain cells that had initially been left empty were filled subsequently with gallium, germanium and technetium, three "new" elements that were discovered thanks to the chemical properties inferred from their positions in the Mendeleev's periodic table. This predictive aspect explains the success of this classification (Photos 1.1 and 1.2).

[^0]| ${ }_{1.00794}$ <br> Hydrogen |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | $\begin{aligned} & { }_{2} \mathrm{He} \\ & 4.0026 \\ & \text { Hélium } \\ & \hline \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \hline{ }_{3} L i \\ & 6.941 \\ & \text { Lithium } \\ & \text { Lithe } \end{aligned}$ | $\begin{gathered} { }_{4} \mathrm{Be} \\ \text { 9.0.01218 } \\ \text { Berylium } \end{gathered}$ |  |  |  |  |  |  |  |  |  |  | $\begin{gathered} \hline{ }_{5} B \\ 10.8110 \\ \text { Boron } \\ \hline \end{gathered}$ | $\begin{aligned} & \hline{ }_{6} C \\ & 12.0107 \\ & \text { Carbon } \end{aligned}$ | $\begin{gathered} \hline{ }_{7}^{7} N \\ 14.0067 \\ \text { Nitrogen } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{8} \mathrm{O} \\ \text { 15.9994 } \\ \text { Oxygen } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{9} F \\ 18,9984 \\ \text { Fluorine } \end{gathered}$ | $\begin{gathered} { }_{10} \mathrm{Ne} \\ \text { 20.1797 } \\ \text { Neon } \end{gathered}$ |
|  | $\underset{\substack{12 M g \\ \text { Magnesium }}}{ }$ |  |  |  |  |  |  |  |  |  |  | $\begin{gathered} \hline{ }_{13} \mathrm{Al} \\ \text { 26.4815} \\ \text { Aluminium } \end{gathered}$ |  | $\begin{gathered} { }_{15} P \\ \begin{array}{c} 30.9738 \\ \text { Phosphorus } \end{array} \end{gathered}$ | $\begin{aligned} & \hline{ }_{16} \mathrm{~S} \\ & \begin{array}{c} 32.065 \\ \text { Sulfur } \end{array} \\ & \hline \end{aligned}$ | $\begin{aligned} & \hline{ }_{17} \mathrm{Cl} \\ & \hline \text { 35,453 } \\ & \text { Clorine } \end{aligned}$ | $\begin{aligned} & \hline 18 \mathrm{Ar} \\ & \text { 39.948 } \\ & \text { Argon } \\ & \hline \end{aligned}$ |
| $\begin{array}{r} { }_{19} K \\ 39.0983 \\ \text { Potassium } \\ \hline \end{array}$ | $\begin{aligned} & \text { 20 } \begin{array}{l} \text { Ca } \\ \text { 4.0.078 } \\ \text { Calcium } \end{array} \\ & \hline \end{aligned}$ | $\begin{gathered} \quad S c \\ \begin{array}{c} 21.9559 \\ 44.959 \\ \text { Scandium } \\ \hline \end{array} ⿳ ⺈ ⿴ 囗 十 一 ~ \end{gathered}$ | $\begin{gathered} { }_{22}{ }^{22} \\ 47.867 \\ \text { Titanium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{23} \mathrm{~V} \\ 50.9415 \\ \text { Vanadium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{24} \mathrm{Cr} \\ 51.996 \\ \text { Chromium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{25} \mathrm{Mn} \\ 54.938 \\ \text { Manganese } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{26}{ }^{26} \\ 5.8 .85 \\ \text { Iron } \\ \hline \end{gathered}$ |  |  | $\begin{array}{r} { }_{29} \mathrm{Cu} \\ 63.548 \\ \text { Copper } \\ \hline \end{array}$ | $\begin{gathered} 30 \mathrm{Zn} \\ 65.409 \\ \text { Zinc } \\ \hline \end{gathered}$ | ${ }_{31} G a$ <br> 69.723 <br> Gallium | $\begin{gathered} \begin{array}{c} { }_{32} \mathrm{Ge} e \\ \text { Germanium } \end{array} \\ \hline \end{gathered}$ | $\begin{array}{r} \begin{array}{r} 33 \\ \hline \end{array}{ }^{33} \\ 74.922 \\ \text { Arsenic } \\ \hline \end{array}$ | $\begin{array}{r} 34 \mathrm{Se} \\ \begin{array}{c} 34.96 \\ \text { Selenium } \end{array} \\ \hline \end{array}$ | $\begin{array}{r} 35 \mathrm{Br} \\ 79,904 \\ \text { Bromine } \\ \hline \end{array}$ | $\begin{array}{r} 36 r \\ 33.798 \\ 8 \text { Kypton } \\ \hline \end{array}$ |
| $\begin{aligned} & \begin{array}{l} 37 \\ \hline \text { 37 } \end{array} \\ & 85.4678 \\ & \text { Rubidium } \end{aligned}$ | $\begin{gathered} \hline 38 S r \\ 87.62 \\ \text { Strontium } \\ \hline \end{gathered}$ | $\begin{gathered} \hline{ }_{39} Y \\ 88.906 \\ \text { Yttrium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{40} \mathrm{Zr} \\ 91.224 \\ \text { Zirconium } \\ \hline \end{gathered}$ | $\begin{aligned} & \hline{ }_{41} \mathrm{Nb} \\ & 9.2906 \\ & \text { Niobium } \\ & \hline \end{aligned}$ | $\begin{gathered} \hline{ }_{42} \mathrm{Mo} \\ 95.94 \\ \text { Molybdenum } \\ \hline \end{gathered}$ | $\begin{array}{\|c\|} \hline{ }_{43} T c \\ 99.00 \\ \text { Technetium } \\ \hline \end{array}$ | $\begin{array}{\|c\|} \hline 44 \\ \hline 14.07 \\ \text { 101.07 } \\ \text { Ruthenum } \end{array}$ | $\begin{gathered} \hline{ }_{45} \mathrm{Rh} \\ \text { 102.905 } \\ \text { Rhodium } \\ \hline \end{gathered}$ | $\begin{array}{r} \hline 46 P d \\ 106.42 \\ \text { Palladium } \\ \hline \end{array}$ | $\begin{aligned} & { }_{47} \mathrm{Ag} \\ & \text { ing } \\ & \text { Siver } \\ & \text { Siver } \\ & \hline \end{aligned}$ | $\begin{aligned} & \hline{ }_{48} \mathrm{Cd} \\ & 112.411 \\ & \text { Cadmium } \end{aligned}$ | $\begin{aligned} & \hline \text { 49 } \text { In } \\ & \text { 114.818 } \\ & \text { Indium } \\ & \hline \end{aligned}$ | $\begin{array}{\|c\|} \hline{ }_{50} S n \\ 118.7110 \\ \text { Tin } \\ \hline \end{array}$ | $\begin{gathered} \hline{ }_{51} \mathrm{Sb} \\ 121.760 \\ \text { Antimony } \\ \hline \end{gathered}$ | $\begin{gathered} \hline{ }_{52} T e \\ 127.60 \\ \text { Tellurium } \end{gathered}$ | $\begin{gathered} \hline{ }_{53} I \\ 126,904 \\ \text { lodine } \\ \hline \end{gathered}$ | $\begin{aligned} & \hline{ }^{54} \mathrm{Xe} \\ & \text { 131.293 } \\ & \text { Xenon } \\ & \hline \end{aligned}$ |
| $\begin{aligned} & \\ & \begin{array}{l} 55 \\ 132.905 \\ \text { Cacsum } \\ \hline \end{array} \\ & \hline \end{aligned}$ | $\begin{aligned} & { }^{56} \text { Ba } \\ & 137.327 \\ & \text { Baryum } \\ & \hline \end{aligned}$ | $\int$ | $\begin{gathered} { }_{72} \mathrm{Hf} \\ 178.49 \\ \text { Hafnium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{73} T a \\ 180.948 \\ \text { Tanalum } \end{gathered}$ | $\begin{gathered} 74 \mathrm{~W} \\ 183.84 \\ \text { Tungsten } \end{gathered}$ | $\begin{gathered} 75 R e \\ \text { 75 } R 2.207 \\ \text { Rhenium } \\ \hline \end{gathered}$ | $\begin{aligned} & { }_{76} \mathrm{Os} \\ & 190.23 \\ & \text { Osmium } \\ & \hline \end{aligned}$ | $\begin{gathered} { }_{77} I r \\ \text { 192.217 } \\ \text { Indium } \\ \hline \end{gathered}$ | $\begin{aligned} & { }_{78} \mathrm{Pt} \\ & \text { 195.078 } \\ & \text { Platine } \\ & \hline \end{aligned}$ | $\begin{gathered} 79 A u \\ \begin{array}{c} 79 \\ \text { 196.966 } \\ \text { Gold } \end{array} \\ \hline \end{gathered}$ | $\begin{array}{r} { }_{80} \mathrm{Hg} \\ 20.59 \\ \text { Mercury } \\ \hline \end{array}$ | $\begin{gathered} { }_{81} T l \\ \text { 204.383 } \\ \text { Thallium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{82} P b \\ \text { 207.2 } \\ \text { Lead } \\ \hline \end{gathered}$ | $\begin{aligned} & { }_{83} B i \\ & 208.980 \\ & \text { Bismuth } \end{aligned}$ | $\begin{aligned} & { }_{84}{ }^{24} \mathrm{Po} \\ & \text { Polonium } \\ & \text { Polonium } \end{aligned}$ | $\begin{aligned} & { }_{85} A t \\ & 210,00 \\ & \text { Astatine } \\ & \hline \end{aligned}$ | $\begin{aligned} & \begin{array}{l} 86 R n \\ 222.00 \\ \text { 22don } \\ \text { Radon } \\ \hline \end{array} ⿳ ⺈ ⿴ 囗 十 一 ~ \end{aligned}$ |
| $\begin{aligned} & \hline{ }_{87} \mathrm{Fr} \\ & 223.00 \\ & \text { Francium } \end{aligned}$ | $\begin{aligned} & \hline{ }_{88}^{88} \text { Ra } \\ & 226.025 \\ & \text { Radium } \\ & \hline \end{aligned}$ | 仡 | $\begin{gathered} \hline{ }_{104} R f \\ 261.00 \\ \text { Rutherfordium } \end{gathered}$ | $\begin{gathered} { }_{105} \mathrm{Db} \\ \overline{-} \\ \text { Dubnium } \end{gathered}$ | $\begin{array}{\|c} \hline{ }_{106} \mathrm{Sg} \\ -\quad- \\ \text { Seaborgium } \end{array}$ | $\begin{gathered} { }_{107} B h \\ -\quad- \\ \text { Bohrium } \end{gathered}$ | $\begin{gathered} \hline{ }_{108} H s \\ -\quad- \\ \text { Hassium } \\ \hline \end{gathered}$ | $\begin{array}{\|c\|} \hline{ }_{109} M t \\ \text { Meiterium } \\ \hline \end{array}$ | $\begin{gathered} { }_{110} \mathrm{Ds} \\ \text { Damstadium } \\ \hline \end{gathered}$ | $\begin{array}{\|c\|} \hline 1111^{2}-- \\ \text { Roengenium } \\ \hline \end{array}$ | $\begin{aligned} & { }_{112} \mathrm{Cn} \\ & -\quad-\quad \\ & \text { Copenicium } \end{aligned}$ | $\ldots$ |  |  |  |  |  |
| Lanthanoids |  | $\underbrace{57} \begin{gathered}\text { La } \\ 138.905 \\ \text { Lanthanum }\end{gathered}$ | $\begin{gathered} { }_{58} \mathrm{Ce} \\ 140.116 \\ \text { Cerium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{59} \mathrm{Pr} \\ 140.908 \\ \text { Praseodymium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{60} \mathrm{Nd} \\ 14.24 \\ \text { Neodymium } \end{gathered}$ | $\begin{gathered} { }_{61} \mathrm{Pm} \\ \hline \text { Promethium } \\ \hline \end{gathered}$ | $\begin{array}{\|c\|} \hline 62 \\ 15 m \\ \text { 150.38 } \\ \text { Samarium } \\ \hline \end{array}$ | $\begin{aligned} & { }^{63} \mathrm{Eu} \\ & 1151.964 \\ & \text { Europium } \\ & \hline \end{aligned}$ | $\begin{gathered} { }_{64} G d \\ 157.25 \\ \text { Gadolinum } \end{gathered}$ | $\begin{gathered} { }_{65} \mathrm{~Tb} \\ 158.925 \\ \text { Terbium } \\ \hline \end{gathered}$ | $\left.\begin{array}{\|c\|} { }_{66} \mathrm{Dy} \\ 162.550 \\ \text { Dysprosium } \end{array} \right\rvert\,$ | $\begin{aligned} & { }_{67} \mathrm{Ho} \\ & 1174.930 \\ & \text { Holmum } \\ & \hline \end{aligned}$ | $\begin{gathered} { }_{68} E r \\ 167.269 \\ \text { Erbium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{69} \mathrm{Tm} \\ \text { 168.934 } \\ \text { Thulium } \end{gathered}$ | $\begin{gathered} { }_{70} \mathrm{Yb} \\ 173.04 \\ \text { Yterbium } \end{gathered}$ | $\begin{gathered} { }_{71} L u \\ 174.957 \\ \text { Lutetium } \\ \hline \end{gathered}$ |  |
| Acti | noids |  <br> $\begin{array}{c}89 \\ 227.00 \\ \text { Actinum }\end{array}$ |  | $\begin{array}{r} { }_{91} P a \\ \text { 231.036 } \\ \text { Protactinium } \end{array}$ | $\begin{gathered} { }_{92} U \\ \text { 238.029 } \\ \text { Uranium } \end{gathered}$ | $\begin{array}{\|c} \hline{ }_{93} N p \\ 237.048 \\ \text { Neppunium } \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline{ }_{94} P u \\ \text { 239.052 } \\ \text { Plutonium } \end{array}$ | $\begin{array}{\|c\|} \hline{ }_{95} \mathrm{Am} \\ 241.057 \\ \text { Americium } \end{array}$ | $\begin{aligned} & \hline{ }_{9} \mathrm{Cm} \\ & \begin{array}{c} \text { 244.063 } \\ \text { Curium } \\ \hline \end{array} \\ & \hline \end{aligned}$ | $\begin{array}{\|c\|} \hline{ }_{97} B k \\ 249 \\ \text { Berkelium } \end{array}$ | $\left\lvert\, \begin{gathered} { }_{98} C f \\ 252 \\ \text { Californium } \end{gathered}\right.$ | $\begin{array}{\|c\|} \hline{ }_{99} E s \\ 253 \\ \text { Einstenium } \end{array}$ | $\begin{array}{\|c\|} \hline 100 \mathrm{Fm} \\ 257 \\ \text { Fermium } \end{array}$ | $\begin{gathered} { }_{101} \text { Md } \\ \text { Mendeckium } \\ \hline \end{gathered}$ | $\begin{gathered} { }_{102} \mathrm{No} \\ 259 \\ \text { Nobelium } \end{gathered}$ | $\begin{gathered} { }_{103} L r \\ 226 \\ \text { Laverexium } \end{gathered}$ |  |
|  |  |  |  |  |  |  |  |  |  |  |  | $\begin{array}{\|c\|} \hline \begin{array}{c} \text { Stomic moss } \\ \text { atome } \\ \text { name } \end{array} \\ \hline \end{array}$ |  |  |  |  |  | ${ }_{1} \mathrm{H}$ Other non－metals，${ }_{3} \mathrm{Li}$ Alkali metals，${ }_{4} \mathrm{Be}$ Alkali earth metals，${ }_{21} \mathrm{Sc}$ Metals，${ }_{5} B$ Metalloids，${ }_{9} \mathrm{~F}$ Halogens，${ }_{2} \mathrm{He}$ Noble gases，${ }_{43} \mathrm{Tc}$

Fig．1．1 Mendeleev＇s periodic table or the periodic table of elements

Photo 1.1 The founding
fathers of the periodic table:
Dmitri Ivanovich
Mendeleev (1834-1907)
(Edgar Fahs Smith
collection, University of Pennsylvania)


Photo 1.2 The founding fathers of the periodic table: Julius Lothar Meyer (1830-1895) (from Wikipedia)


The noble gases, discovered later, were placed in the last column afterwards, resulting in the table in the form known today. Without entering into a detailed chemical description of all the elements, the following should be noted:

- The hydrogen atom is the main constituent of the universe, not to be confused with hydrogen gas, $\mathrm{H}_{2}$, which consists of two hydrogen atoms.
- The rare (or noble) gases ( $\mathrm{He}, \mathrm{Ne}, \mathrm{Ar}, \mathrm{Xe}, \mathrm{Kr}, \mathrm{Rn}$ ) are located in the last column to the right. These gases are very stable from a nuclear standpoint, they are not chemically reactive, and are very difficult to liquefy.
- The alkali metals, $(L i, N a, K)$ are located in the first column. These are highly electropositive metals. They have a low density and are soft metals that are chemically highly reactive. They are known as powerful reducers.
- The lanthanides ( $C e, P r$ ) are generally strong neutron absorbers. This family includes rare earth metals, chemical elements that are found in only minute
quantities on Earth, such as samarium, gadolinium and erbium, which have strong neutron-absorbing isotopes.
- The halogens, or "salt-formers", $(F, C l, B r, I)$ are highly electronegative and are found in the penultimate column. Generally very corrosive, they are powerful oxidants.
- The transuranic or transuranium elements form a family of chemical elements beyond uranium and are sometimes referred to somewhat confusingly as heavy nuclei: the term heavy nuclei is taken by some as the name for chemical elements beyond lead and this broader definition encompasses the transuranic elements.

The relative abundance of elements in the universe, which decreases as their mass increases, is explained by nucleosynthesis (as first approximation), i.e. the production of heavy nuclei by fusion in the cores of stars (Annual Review of Nuclear Science, Vol. 2, 1953, p. 1).

### 1.2 Molecules

(Mahan et al. 1970; Joven-Alvarez 2015)
In 1661, the Anglo-Irish chemist and physicist, Robert Boyle, son of the Duke of Cork, published The Sceptical Chymist, which broke with the tradition of magic and alchemy in the chemistry of old times. Boyle was convinced that elements such as gold cannot be created by man, as the alchemists held, but only by Nature. He believed that all matter is composed of basic elements that combine to form substances, and that air is composed of molecules that "float" in a vacuum "like flies". The elements do indeed combine in nature to form molecules. For example, hydrogen gas contains $H_{2}$ molecules each consisting of two hydrogen atoms.

Antoine de Lavoisier ${ }^{3}$ (1743-1794), universally known for his law of conservation of matter, published during the French Revolution, described how elements combine. However, this was J.D. Richter who gave the basis of the law of multiple

[^1]proportions (Wurtz 1904, p. 7). In 1794, J.L. Proust ${ }^{4}$ supported the idea that a compound can only be created by a fixed combination of elements: the ammonia molecule, $\mathrm{NH}_{3}$, contains one atom of nitrogen, N , and three atoms of hydrogen, H . The law of definite proportions or Proust's law establishes that if an element $A$ combines with another element $B$, the ratio of masses $A / B$ is constant. This

(Metropolitan Museum of Art)
${ }^{4}$ Joseph Louis Proust (1754-1826) was a French chemist; he was named Chief of the Salpêtrière Hospital pharmacy (Paris) in 1775 and joined the Academy of Sciences in 1816. He successfully synthesized sugar from grapes and defined the law of definite proportions published in 1794, which makes him one of the precursors of atomic theory.
remains true if $A$ combines with another element $C$ or $D$, in which case $A / C$ and A/D will be fixed, but with different constant values (Mahan et al. 1970, p. 6).

Richter established that if element $B$ combines with $C$ or $D$, then it is the same quantities of $C$ or of $D$ that combined with $A$ which will also combine with $B$. This is the law of multiple compositions. In 1811, the Italian physicist Amedeo Avogadro (1776-1856) accurately defined the term molecule and its relationship to atoms (Mahan et al. 1970, p. 9). The English chemist and physicist John Dalton (1766-1844, Fig. 1.2) resuscitated the ancient theory of Democritus according to which matter is made up of indivisible atoms (Wurtz 1904, p. 2). He understood that the characteristics of the atom helped to explain why only a fixed combination of oxygen and hydrogen leads to the synthesis of water: one volume of oxygen added to two volumes of gaseous hydrogen forms water, which is a compound, or a combination of atoms in the form of a molecule. John Dalton, like Proust, distinguished between chemical compounds and mixtures of substances and established a classification based on atomic weight.

### 1.3 Isotopes

Between 1910 and 1912, studies by Frederick Soddy, ${ }^{5}$ Rutherford's pupil at the McGill Institute in Montréal, followed by the experimental proof furnished by Joseph John Thomson (1856-1940) and his assistant F.W. Aston (1877-1946), revealed atoms of different masses having identical chemical properties. In 1913, the term isotope was used for the first time by Frederick Soddy in an article in Nature: a single chemical element may thus occur in the form of several different


[^2]Fig. 1.2 John Dalton, a child prodigy who became a school director at the age of 19 , collected more than 200,000 weather measurements during his lifetime, making him one of the forerunners of the modern science of meteorology (The Robinson library)


Photo 1.3 Frederick Soddy (1877-1956), photo taken around 1902, public domain

isotopes having different atomic masses, but occupying the same cell in the periodic table (Photo 1.3).

This overturned the theory of English physicist William Prout (1785-1850) according to which the atomic mass of any element is a whole multiple of that of

Table 1.1 Relative isotopic abundance of argon and potassium

|  |  | Numbers of weight and abundance |  |  |  |  |  | Element |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | Atomic number atomic weight |  |  |  |  |  |  |  |
| Argon (A) | 18 | 36 | 37 | 38 | 39 | 40 | 41 |  |
| Potassium (K) | 19 | 0.3 |  | 0.06 |  | 99.6 |  | 39.9 |

Based on strict order of weight, the places of argon and potassium in the periodic table should be inverted
hydrogen (Fernandez 2006, p. 187), but which could not account for the atomic mass of chlorine (35.5). Indeed, natural chlorine comprises isotopes of different masses. It now became possible to explain the chemical enigma of the inverted position in the periodic table of tellurium (mass 127.6) and iodine (mass 126.9). In terms of order of atomic weights, they could not be placed in the proper columns within the table on the basis of their chemical properties. J.J. Thomson ${ }^{6}$ provided experimental proof of the existence of isotopes in 1912. On inspecting the tracks in the form of parabolas resulting from the impact of neon ions (gaseous residue of liquid air) deviated in an electric field, Soddy noted a lighter track which he attributed to ionized neon 22 and which differed from the track for neon 20. Table 1.1 gives relative isotopic abundances of Argon and Potassium.

Aston confirmed this result in 1919 using his mass spectrometer, which clearly indicated the existence of two types of neon atom in natural neon gas (atomic weight: 20.2): ${ }_{10}^{20} \mathrm{Ne}$ (approximately $90 \%$ ) and ${ }_{10}^{22} \mathrm{Ne}$ (approximately 10\%). Later, a third nucleus, ${ }_{10}^{23} \mathrm{Ne}$, was discovered in the form of traces. These different atoms are known as isotopes. The term isotopic abundance is used to designate the proportion of different isotopes of a single natural element. For most chemical bodies, abundance on earth is globally constant. However, for certain chemical elements that continue to be formed (e.g. lead, which constitutes the final phase of disintegration of uranium), local abundance depends (weakly) on enrichment of the substrate in radioactive nuclei. Thus, the atomic weight of natural lead ranges from 206.01 for lead from Norwegian cleveite, to 207.9 for lead from thorite (also from Norway). One hypothesis advanced to explain local changes in isotopic abundance is the possibility of elements being carried to Earth in meteorites of a different age to our planet. Isotopes of the same element $X$ are thus distinguished by different atomic weights $A$. An isotope is fully defined by a notation having the following form: ${ }_{Z}^{A} X$. There are 280 naturally occurring stable isotopes and some 50 natural radioactive isotopes. Note that an isotope may be both natural and radioactive.

[^3]
### 1.4 Atoms

(Guillien 1963; Halliday 1957; Evans 1955; Filippi 1965; Steigler 1966)
In 1911, Ernest Rutherford ${ }^{7}$ carried out a landmark experiment involving the diffraction of $\alpha$ particles using a piece of gold foil (Fig. 1.3). He noted some


Fig. 1.3 Deflection of $\alpha$ particles using gold foil (1911)
${ }^{7}$ Ernest Rutherford (1871-1937) was an exceptionally gifted physicist from New Zealand. His talents being recognized at an early age, he left for England to complete his scientific studies at the highly renowned Cavendish Laboratory in Cambridge, under the direction of J.J. Thomson, and he specialized in experimental physics. In 1898, he was offered the chair of physics at the McGill capital Institute in Montréal (Canada), where he developed experimental methods designed to study ionization and radioactivity. He identified the nature of $\alpha$ radiation. In 1907, he returned to Manchester, where he became the father of nuclear physics with this discovery in 1911 of the atomic nucleus. He was awarded the Nobel Prize in 1908 and directed the Cavendish Laboratory from 1919. He was relatively uninterested in theoretical physics and had a jovial and completely unpretentious character, coining such phrases as "All science is either physics or stamp collecting".


Ernest Rutherford in 1908, Public domain
deflection of the $\alpha$ particles (around one particle in 8000 was deflected from the straight path). These "ricochets" were due to repulsion of the positive charges on the $\alpha$-particles by a positive charge within the atomic nuclei (Rival 1996, p. 123).

Rutherford's atomic firing range involved the use of a source of radium 226 placed inside a drilled lead box serving as a "canon" that fired only $\alpha$ particles emitted in the direction of the hole at the gold foil (the other $\alpha$ particles were stopped by the lead). The $\alpha$ particles passed through a piece of gold foil placed in front of a luminescent screen enabling the impact of any deflected $\alpha$ particles to be viewed. Rutherford showed by calculation that such deflection can only be explained if the entire positive charge was concentrated in a very small area at the center of the atom: the so-called nucleus. The atom thus comprises a very dense nucleus ( $10^{17} \mathrm{~kg} / \mathrm{m}^{3}$ ) containing $Z$ protons having a positive charge (+1.6 $10^{-19}$ Coulomb) and $N$ neutrons without charge ( $N=A-Z$ ), as well as an electron cloud of $Z$ electrons having a negative charge ( $-1.6 \quad 10^{-19}$ Coulomb), and negligible but not zero mass, spinning around the nucleus at extremely high speed. The radius of the atom, including the electron cloud, is of the order of $10^{-8} \mathrm{~cm}$. The radius of the nucleus is around $r_{0} \cdot A^{1 / 3}$ Fermi, a recent subunit within the metric system ${ }^{8}$ (symbol $F, 10^{-15}$ metre $=1 \mathrm{fm}$ ) with $r_{0} \approx 1.3-1.5 \mathrm{fm}$, or around $10^{-12} \mathrm{~cm}$ to give some idea. In their normal state. Standard atoms are electrically neutral as the number of electrons is equal to the number of protons. Where the electrostatic equilibrium is broken by a smaller or greater number of electrons, we speak of ions. In the same way that isotopes are atoms having the same atomic number $Z$ (e.g. ${ }_{10}^{20} \mathrm{Ne}$ and ${ }_{10}^{22} \mathrm{Ne}$ ), isobars are atoms with the same atomic weight $A$ (e.g. ${ }_{8}^{15} O$ and ${ }_{7}^{15} N$ ). Isomers designate two isotopes having the same values for $A$ and $Z$, but having a different state of excitation (e.g. ${ }_{95}^{242} \mathrm{Am}$ and the metastable ${ }_{95}^{242 m} \mathrm{Am}$ ).

[^4]
### 1.5 Avogadro's Number



An Italian postage stamp of Amedeo Avogadro bears his traditional image (The Marguet collection)
In 1811, Amedeo Avogadro di Quaregna (1776-1856), a physics professor at the University of Turin (Italy), formulated the hypothesis that equal volumes of different gases contain the same number of molecules at equivalent temperature and pressure (known as the Avogadro's law). According to Avogadro, $\mathrm{H}_{2} \mathrm{O}$ is a molecule (literally, a "small mass"), i.e. the smallest possible particle of water. He distinguished such particles clearly from atoms, the ultimate indivisible particle. If $1 \mathrm{~cm}^{3}$ of hydrogen contains as many atoms as $1 \mathrm{~cm}^{3}$ of oxygen, and since $1 \mathrm{~cm}^{3}$ of oxygen weighs 16 times more than $1 \mathrm{~cm}^{3}$ of hydrogen, an oxygen atom must be 16 times heavier than a hydrogen atom. Avogadro's hypothesis was subsequently verified. Avogadro's number characterizing the quantity of atoms per mole is represented by $\mathcal{N}$ (Photo 1.4).

In 1814, André-Marie Ampère, famous for his pioneering work in the field of electrodynamics, noted that the volumes developed by the respective molecular masses of various ideal gases were the same, namely 22.4 liters, under normal temperature and pressure conditions. In 1875, the physicist Johannes Diderik Van der Walls proposed the first value of Avogadro's constant, with fairly respectable accuracy for the time:

$$
10^{23} \mathrm{~mol}^{-1}<\mathcal{N}<10^{24} \mathrm{~mol}^{-1}
$$

Many measuring methods have since been proposed: measurement of the Brownian motion of particles immersed in water (Jean Perrin), blackbody radiation, diffusion of light by gases, x-ray diffraction, the volume of helium produced by alpha radioactivity, etc. All of these experiments confirm the value of $\mathcal{N}$ as lying close to $610^{23} \mathrm{~mol}^{-1}$. One especially precise and relatively simple measurement consists in directly measuring the distance of reticular planes (containing the positions of atoms) in a crystal of NaCl by means of x-ray diffraction. When x-rays travelling through a vacuum strike a substance, they are deflected from their normal path at the interface between the vacuum and the substance. For this type of wavelength, materials have a refractive index slightly below 1 . Beyond a threshold angle, the rays are totally reflected. This threshold angle is always around $90^{\circ}$, enabling x-ray reflection to be observed at a grazing incidence. The parameter


Par A. AVOGADRO.

## I.

M. Gay-Lussac a fait voir dans un Mémoire intéressant (Mémoires de la Sociélé d'Arcueil, tome II) que les combinaisons des gaz entre cux se font toujours selon des rapports très-simples en volume, et que lorsque le résultat de la combinaison est gaxeux, son volume est aussi en rappont très-vimplo avec celui de ses composans; mais les rapports des quantités de substances dans les combinaisons ne paroissent pouvoir dépendre que du nombre relatif des molécules qui se combinent, et de celui des molécules composées qui en résultent. Il faut donc admettre qu'il y a aussi des rapports très-simples entre les volumes des substances gazeuses, et le nombre des molécules simples on composées qui les forme. L'hypothése qui se présente la première à cet égard, et qui paroít même la seule admissible, est de supposer que le nombre des molécules intégrantes dans les gaz quelconques, est toujours le méme à volume égal, ou est loujours proportionnel aux volumes. En eflet, si on supposoit que le nombre des molécules contenues dans uu volume donné fatt différent pour les différens gaz, il ne scroit guère possible de concevoir que la loi qui présideroit à la distance des molécules, pat.donner, en tout cas, des rapports aussi simples que les faits que nous venons de citer, nous obligent à admettre entre le volume et le nombre des molécules. Au contraire, on

Photo 1.4 First page of Avogadro's paper, "Essai d'une manière de déterminer les masses relatives des molécules élémentaires des corps, et les proportions selon lesquelles elles entrent dans ces combinaisons" [Test of a method of determining the relative masses of elementary particles of bodies, and their proportions within these combinations], Journal de Physique et de Chimie, Tome LXXIII, pp 58-76, July 1811 (The Marguet collection)
$a$ of the lattice of the cubic crystal of NaCl has been determined by the study of Bragg spectra as $a=5.6402 \AA$. Each lattice in the crystal comprises 8 elementary cubes. The lattice contains 8 chlorine atoms at the 8 summits of the lattice, 6 chlorine atoms at the centers of the 6 sides of the lattice, 1 sodium atom at the center of the lattice and 12 sodium atoms at the center of the 12 edges of the lattice. But each atom is part of 8 cubes in contact with either a side or an edge. On average, one single complete atom may be associated per elementary cube having an edge of $a / 2=2.8201 \AA$. The molar mass (molecule-gram) of NaCl , i.e. $58.443 \mathrm{~g} / \mathrm{mol}$, contains $2 \mathcal{N}$ atoms, half of which are sodium and the other half chlorine. The


Fig. 1.4 Deflection of x-rays by a cube of NaCl crystal
density of rock salt is $2.1632 \mathrm{~g} / \mathrm{cm}^{3}$ at $20^{\circ} \mathrm{C}$. The volume occupied by one mole of rock salt is given by:

$$
V=2 \mathcal{N}\left(\frac{a}{2}\right)^{3}=\frac{M}{\rho}
$$

The numerical application of this formula can be used to obtain a value of $6.022992210^{23} \mathrm{~mol}^{-1} \pm 0.001$ which is consistent with the more accurate value known today (Fig. 1.4).

In 1971, the General Conference on Weights and Measures defined a new base unit for matter: the mole (symbol mol in the International System ${ }^{9}$ ). One mole of carbon 12 contains $\mathcal{N}$ atoms of carbon, i.e. $6.02210^{23}$ atoms. Since one mole of carbon 12 weighs 12 grams, a carbon atom weighs $12 / \mathcal{N}$. i.e. around $210^{-23}$ grams. The value of Avogadro's number is today known with great precision:

$$
\mathcal{N}=6.022136710^{23} \mathrm{~mol}^{-1} \pm 5.9 \quad 10^{-5} \%
$$

The well-known French physicist and experimenter Jean Perrin, ${ }^{10}$ a great partisan of atomistic theory, endeavored to calculate Avogadro's number with the

[^5]Photo 1.5 Jean Perrin (1870-1942) One of the founding fathers of atomic theory, (Public domain)

greatest possible precision (Bloch 1958, p. 99). By 1913, he had already obtained no less than 13 values using entirely different procedures, and the consistency of the results definitively removed all doubts about the reality of the existence of molecules, despite the fact that they could not be viewed by any existing apparatus at the time (Photo 1.5).

Among the experimental methods used by Jean Perrin, we may single out two procedures developed in 1909. The first involves immersing an emulsion of perfectly spherical grains of known size in a liquid. Perrin prepared this emulsion using gutta percha, a type of latex for which he was able to control the coagulation and produce spherules of known size. Perrin then demonstrated that these spherules, which continued to be visible suspended in water, followed trajectories describing broken lines. The changes in trajectory resulted from collision between the spherules and water molecules subject to Brownian motion. By precise measurement, he showed that the distribution of the spherules obeyed a Laplace law axially, namely that when the heights of an emulsion in a container follow an arithmetical law, the number of spherules in suspension conversely follows a geometric progression. At equilibrium, the action of gravity (from which must be subtracted Archimedes' buoyant force) is compensated for by osmotic pressure, i.e. the action of diffusion induced by Brownian motion. Perrin used the Boltzmann relationship (which we will examine later) of distribution of the population of spherules $n(T, h)$ at a given temperature, as a function of total energy to express the phenomenon in the following mathematical formula:

[^6]$$
\frac{n\left(T, h_{2}\right)}{n\left(T, h_{1}\right)}=\frac{e^{-\frac{\frac{3}{2} k T+m g h_{2}}{k T}}}{e^{-\frac{\frac{3}{2} k T+m g h_{1}}{k T}}}=e^{-\frac{m g\left(h_{2}-h_{1}\right)}{k T}}
$$

The term $3 k T / 2$, where $k$ is Boltzmann's constant, corresponds to the kinetic energy of the spherule ( $k T / 2$ for each of the 3 degrees of freedom in a 3-D space), while the term $m g h$ describes the potential energy of the spherule as a function of its altitude). He used the law of axial distribution of the number of spherules in an isothermal container:

$$
n(T, h)=n_{0} e^{-\frac{m_{g} h}{k T}}
$$

This law is identical to the exponential law of decreasing pressure in a column of gas at uniform temperature. By measuring Boltzmann's constant in this way, Perrin was able to measure Avogadro's number having established the constant for ideal gases at $R=8.31 \mathrm{~J} . \mathrm{mol}^{-1} . \mathrm{K}^{-1}$, which was easy to obtain using macroscopic measurements based on the law of ideal gases:

$$
\mathcal{N}=\frac{R}{k} \approx 6.8510^{+23} \mathrm{~mol}^{-1}
$$

Jean Perrin's second approach was equally interesting. He used Einstein studies on Brownian motion proving that the diffusion coefficient is related to mean quadratic displacement by the following relationship:

$$
\left\langle r^{2}\right\rangle=2 d D t
$$

where $r$ is the distance of displacement along a straight line between two collisions, $d$ is the dimensional of the problem (i.e. 3 in 3D geometry), $D$ is the diffusion coefficient and $t$ is time. The diffusion coefficient is given by:

$$
D=\frac{R T}{\mathcal{N} 6 \pi a \eta}
$$

where $a$ is the radius of the spherules and $\eta$ is the viscosity of the liquid. Thus, with great patience, Jean Perrin measured on graph paper the successive displacements of spherule in order to calculate $\left\langle r^{2}\right\rangle$ as a function of time. Once more, this method gave him a value of around $610^{+23} \mathrm{~mol}^{-1}$.

Note that a precise determination of Avogadro's number may be obtained by means of x-ray diffraction in a crystal lattice (Born 1971, p. 29).

### 1.6 Mass-Energy Equivalence

The early twentieth century was buzzing with ideas about the possibility of inertia associated with energy. Already in 1881, JJ Thomson attributed to a conductor an additional mass of $\Delta m=3 E /\left(4 c^{2}\right)$ where $E$ is the energy of the electrostatic field. In 1900, on observing that the ratio of Poynting energy flux to the electromagnetic impulsion was $1 / c^{2}$, Henri Poincaré suggested that electromagnetic energy must have an apparent mass such that $E=m c^{2}$. From this, he concluded that a Hertzian (radio) emitter giving out energy in wave form must undergo a recoil effect similar to that of cannon on firing a cannon ball (Arzeliès 1966, p. 68). In 1904, Friedrich Hasenöhrl ${ }^{11}$ showed that if we consider the movement of a box with reflective walls containing no matter but containing electromagnetic radiation having a total energy of $E$, because of the pressure of radiation, the latter will behave as if it had a mass of $3 E /\left(4 c^{2}\right)$ (Born 1971, p. 60; Arzeliès 1966, p. 69), but his calculation turned out to be erroneous. Probably the most famous formula in physics, namely the massenergy equivalence formula, was finally demonstrated and re-situated in a highly general context by Albert Einstein (1879-1955) in his theory of Special Relativity, published in 1905 in the German journal 'Annalen der Physik' (Hoffmann 1975; Génie de la science $\mathrm{n}^{\circ} 11$ 2002). The formula states that all types of energy possess

[^7]

Friedrich Hasenörhl (Photo Österreichische-Zentralbibliothek für Physik, Public domain)
inertia, and thus equivalent mass, that may be calculated by dividing the energy by the square of the speed of light in a vacuum:

$$
\begin{gather*}
\text { Einstein's formula (1905): } E=m c^{2}  \tag{1.1}\\
c=2.9979245810^{8} m \cdot s^{-1} \pm 310^{-7} \%
\end{gather*}
$$

According to this formula, 1 kg of matter corresponds to an energy of $8.98348210^{16}$ Joules, with the Joule being the official unit of energy (Photo 1.6).

The story goes that the principle of inertia of energy was discovered independently at the same time by Paul Langevin (1872-1946) and Albert Einstein, according to Marcel Tournier, who was first Langevin's pupil and then his assistant (Langevin 1971): "Developing the consequences of the theory on dynamics, he discovered the fundamental relationship of the inertia of energy. He showed his calculations to his friend, Jean Perrin, who was unable to credit the extraordinary novelty of the result. This made Langevin hesitate; he delayed publishing his findings, which were published only several months later by Albert Einstein". Paul Langevin was not a man motivated by fame, and he never attempted to prove that he was the first to light upon an idea that he had not published.

However, he worked tirelessly to emphasize the work of Einstein in France (Borella 1998). Paul Langevin subsequently specialized in the theory of electromagnetic dynamics and was elected to the Academy of Sciences in 1934. Given the extremely low mass of atoms, it was relatively difficult to use SI units (International System units ${ }^{12}$ of meter-kilogram-second or $M K S$ ) or CGS (centimeter-gram-second). It was therefore decided to define a unit of atomic mass that was simpler to use. Up to 1960, the reference unit used was $1 / 16$ of the atomic weight of a true atom of oxygen- 16 containing 16 nucleons $\left({ }_{8}^{16} O\right)$ (Jouguet 1964, p. 210). This mass unit was thus equivalent to $1.6598310^{-27} \mathrm{~kg}$. However, in chemistry, the historical unit used was $1 / 16$ of the mean mass of natural oxygen (the unit generally used by chemists). In fact, natural oxygen contains several isotopes of oxygen ( ${ }_{8}^{16} \mathrm{O},{ }_{8}^{17} \mathrm{O}$ and ${ }_{8}^{18} O$ ), and the units used by chemist thus differed from those used by physicists. After 1960, it was decided to unify the systems by taking as the reference $1 / 12$ of the mass of the atom ${ }_{6}^{12} C$ (a neutral way of solving the problem!), one mole of which by definition weighs 12 grams. The unified mass unit, u, often referred to as the atomic mass unit (amu) in everyday language (strictly speaking, the amu was based on the old definition relating to oxygen), is equivalent to $1.660540210^{-27} \mathrm{~kg}$. Using Einstein's formula, mass (normally given in kg ) may be expressed as units of energy divided by the square of the speed of light in a vacuum, i.e. in $\mathrm{MeV} / \mathrm{c}^{2}$. Using this approach, it is possible to rapidly calculate energy balance by using the masses expressed in this way since given mass is always multiplied by $c^{2} .1 \mathrm{~kg}$ corresponds to $5.60986110^{29} \mathrm{MeV} / \mathrm{c}^{2}$, and the unified atomic mass unit is thus:

[^8]

Photo 1.6 The famous volume 17 of the 'Annalen der Physik' in which Einstein's original article on relativity was published (The Marguet collection)

$$
1 u \equiv 1.660540210^{-27} \mathrm{~kg} \pm 5.910^{-5} \%=931.54 \mathrm{MeV} / \mathrm{c}^{2}
$$

The atomic mass of an atom, conventionally denoted by $A$, is the whole number closest to the mass of the atom expressed in unit $u$, while the atomic weight is a real
number that may be counted in fractions of $u$. As a first approach, it is reasonable to take the whole number $A$ as the atomic mass for simplified engineering calculations. For the hydrogen atom ${ }_{1}^{1} H$, the atomic mass number $A$ is 1 and its atomic weight is 1.00797 u or $938.924 \mathrm{MeV} / \mathrm{c}^{2}$.

### 1.7 Neutrons

(Alexandrov 1992)
Neutrons were officially discovered by James Chadwick (1891-1974) in 1932, although their existence had already been postulated in 1920 by Ernest Rutherford (see also Photo 1.7). After many years of research, Chadwick correctly interpreted an experiment by Irène and Frédéric Joliot-Curie that involved firing a beam of $\alpha$ particles at beryllium nuclei (Photo 1.8) (Renault 1948, p. 129; Kahan 1963, p. 59):


Photo 1.7 Advertisement of 28 July 1925 on the cover of issue No 127 of "L'Antenne TSF". This French popular science journal ("The bestselling publication on radio technology"!) presented news in the field of radio broadcasting, then at the height of its popularity. There was much talk therein about rationalization of the airwaves by state intervention. However, this advertisement for Neutron synthetic crystals for galena crystal radios, produced by the British company Neutron Ltd in London and distributed in France by Créo, shows that the term "neutron" was already in use at this time and represented by images of radiating material. Although the neutron had not yet been discovered, its name already sparked imaginations! (The Marguet collection)


Photo 1.8 James Chadwick was knighted in 1945 by the King of England. On the right is a stamp of the Maldives in his honor (Public domain and the Marguet collection)

$$
{ }_{2}^{4} \mathrm{He}+{ }_{4}^{9} \mathrm{Be} \rightarrow{ }_{6}^{12} \mathrm{C}+{ }_{0}^{1} n
$$

In 1932, Jean-Louis Destouches ${ }^{13}$ wrote the first book on neutron transport in the French language (Destouches 1932), which provided an extremely clear and particularly perspicacious summary of existing knowledge concerning this new particle (Photo 1.9).

It demonstrates that neutrons cannot be represented as "close" proton-electron pairs, and already postulates the idea of a neutron comprising a positively charged central part surrounded by a negative "atmosphere" of varying density according to the radius, with the entire unit being of spherical symmetry and externally neutral. The penetration of matter by neutrons is discussed in the book using linear attenuation coefficients inversely proportional to the speed of the neutrons, as are

[^9]the effective macroscopic sections, which we shall define in Chap. 2. The most recent data indicate that the mass of the neutron is $1.0086654 \mathrm{u}=1.674928610^{-27}$ kg , i.e. $939.56564 \mathrm{MeV} / \mathrm{c}^{2}$ at rest (Alexandrov 1992, p. 31). The neutron is a nucleon carrying no electric charge, making it the particle of choice as a projectile for bombardment of nuclei (it has no Coulomb barrier resulting from electrostatic forces to be overcome prior to collision with the nucleus). More precisely, although globally neutral, neutrons have a magnetic moment $\mu=-(1.935 \pm 0.02) \mu_{N}$ where $\mu_{N}=e \hbar /\left(2 m_{p} c\right)=5.05110^{-27}{\mathrm{~J} . \mathrm{T}^{-1}}^{(A l e x a n d r o v ~ 1992, ~ p . ~ 63), ~ p r o v i n g ~ t h a t ~ t h e r e ~}$ is an internal distribution of charge. It may therefore interact with unpaired electrons (i.e. electrons not forming part of an electron pair) within electron clouds.

Neutrons have a radius of around 1.3 fm . Free neutrons emit $\beta^{-}$radiation and decay in accordance with the following equation:

$$
{ }_{0}^{1} n \rightarrow{ }_{1}^{1} p+{ }_{-1}^{0} e^{-}+783 \mathrm{keV}
$$

with a half-life of $10.37 \pm 0.06$ minutes (Alexandrov 1992, p. 58).
The De Broglie (1892-1987) wavelength of the neutron is of the order of size of the interatomic distance, accounting for the interference effects, as with electrons (Born 1971, p. 66), that occur when neutron waves are diffracted in crystals. Moreover, this is an extremely useful method of investigation of matter that is utilized in certain cases. Neutrons have a kinetic moment characterized by spin equivalent to that of the proton or the electron. Their associated spin is $1 / 2$ in $\hbar$ units (Alexandrov 1992, p. 33).


Jean-Louis Destouches in 1950 (The Marguet collection, photograph unknown)


Photo 1.9 The first book on neutron transport in the French language by Jean-Louis Destouches (1932, The Marguet collection)

### 1.8 Electrons

(Boutry 1962, p. 197)
In a famous experiment conducted in 1891, the English chemist and physicist William Crookes (1832-1919) discovered the effects of electricity by introducing

Fig. 1.5 Crookes tube


Fig. 1.6 Coolidge tube

an anode connected to the positive terminal of a battery and a cathode in a vacuum tube (Crookes tube). When the cathode is connected to the negative terminal of the battery, a greenish light appears at the bottom of the tube as a result of electrons striking the base of the tube. The German physicist Eugen Goldstein (1850-1930) had the idea of placing a Maltese cross in the path of the electrons and noticed that the shadow of the cross was cast on the bottom of the tube. It was by rotating a wind-milling shaped cross rapidly that Crookes demonstrated the particle nature of electron flux.

Crookes tubes quickly came to be used in the format shown in Fig. 1.5 to produce electrons by x-ray collisions on an anti-cathode, which we shall study below. The concave shape of the cathode allows the electrons to be concentrated at a point on the anti-cathode, heating the latter considerably. This system was improved by Coolidge (Fig. 1.6) with production of electrons via a thermo-ionic effect by heating a tungsten filament by Joule effect and controlling the current used to heat the cathode by means of a rheostat. The heat in the anti-cathode target resulting from the kinetic energy of the electrons is evacuated by means of an array of external cooling fins.

The term 'electron' was first coined by the Anglo-Irish physicist George Stoney (1826-1911) in 1894, but it was officially introduced in 1897 by Joseph John

Photo 1.10 Joseph John Thomson was a brilliant physicist renowned in his time. His numerous pioneering studies on the nature of electricity earned him the Nobel Prize for physics in 1906 (steel engraving of 1896, from Wikipedia, Public domain)


Thomson (1856-1940), director of the famous Cavendish Laboratory (Photo 1.10) (Filippi 1965, p. 183).

Electrons are negatively charged particles. A basic measurement of the charge, the absolute value of which is denoted by " $e$ ", was made by H.A. Wilson in 1903, but it was measured with great precision in the very famous oil drop experiment conducted in 1909 by Millikan (1868-1953), who was awarded the Nobel Prize in 1923 (Filippi 1965, p. 174; Mahan et al. 1970, p. 400). It also figured as a key element in Thomson's "plum pudding" model of the atom consisting of a uniform "sea" of positive charge containing negatively charged electrons. This initial model was found to be erroneous following the discovery of protons at the center of the nucleus, due to Rutherford. The charge carried by electrons, which was measured by Robert A. Millikan using charged drops of oil released vertically through an electrostatic field, is: $-e=-1.60217733 \times 10^{-19} \pm 0.0003 \%$ Coulomb. This charge is negative by convention following a historic error concerning the direction of displacement of electrons in a current within a conductor. The energy acquired by acceleration of an electron subjected to a potential difference of 1 Volt is the definition of the electron-Volt. $1 \mathrm{eV} \equiv 1.6021773310^{-19} \mathrm{~J}$, a unit of energy that does not belong to the international system but which is simpler to use in nuclear physics (Mayo 1998, p. 21). The mass of an electron, classed as a member of the family of light particles, the leptons, is $9.10903897 \times 10^{-31} \mathrm{~kg}$, i.e. 0.00054858 u or 0.511 MeV at rest. Its spin is $1 / 2$ in $\hbar$ units. Electrons are represented by the following notation: ${ }_{-1}^{0} e^{-}$. Note that the electron is a particle with around 2000 times less mass than the neutron and that its mass is often neglected in engineering calculations. It must be remembered that in principle, electrons are not smaller in size than neutrons, despite what one might be led to believe by their mass and by the standard representation of electron shells in textbooks. Although no experiments have ever determined the precise size of an electron, it is generally attributed a radius of $2.8210^{-15} \mathrm{~m}$ (Filippi 1965, p. 190). We speak of the classical radius of the electron, which corresponds to the effective circular section measured in classical electromagnetic theory by making an electron vibrate by means of incident radiation. Electrons have a kinetic moment of rotation around their axis
characterized by spin (Born 1971, p. 141; Peaslee and Mueller 1955, p. 257). Electrons also have a magnetic moment, which plays a key role in quantum physics. Classical electron theory is described in detail in (Becker 1938).

### 1.9 Protons

In 1910, the German physicist Johannes (Hans) W. Geiger (1882-1945) and the New Zealand physicist Ernest Marsden (1889-1970), both students of Rutherford, interpreted the results of experiments involving the scattering of $\alpha$ particles $(z=2)$ using thin targets (thin sheets of gold foil, $Z=79$, (Dodd 1984, p. 5) and deduced the following: "The number of positively charged elementary particles is approximately equal to half the mass number, $A$, of the atom". Analysis of the angle of deflection showed that the charge to be concentrated in the nucleus (by calculating the minimum approach distance $z Z e^{2} /\left(4 \pi \varepsilon_{0} E_{\alpha}\right)$ which is of the order of 40 fm for $z_{\alpha}=2$ and $Z_{\text {gold }}=79$, in other words far less than the size of an atom) and not distributed throughout a sphere of the size of the atom, as postulated in Thomson's model. Analysis of the angle of deflection enabled determination of the charge within the nucleus. The charge on the proton is in fact $+e=+1.602177310^{-19}$ Coulomb. Its mass is $1.672623110^{-27} \mathrm{~kg}$, i.e. 1.0072765 u or 938.273 MeV at rest (lighter than the neutron). The proton is a nucleon having spin of $1 / 2$ in $\hbar$ units. The protons within the nucleus repel one another through Coulomb (electromagnetic) interaction, but the nucleus remains bound together by the strong interaction or strong force (which is around 1000 times stronger than electromagnetic interaction!) (Valentin 1982a, b, p. 41). Further, this force acts indifferently on all hadron particles, and thus between all nucleons, whether charged (protons) or neutral (neutrons), although this force has an extremely short range (of around 1.5 fm ). The proton is designated ${ }_{1}^{1} p$, but since it also constitutes the nucleus of the hydrogen atom, it is occasionally written as ${ }_{1}^{1} H^{+}$. The mass of the proton is practically equal to that of the neutron and this simplification is frequently used in industrial calculations. According to our current state of knowledge, protons appear stable in the free state as far as we know. The proton has a kinetic moment of spin equal to that of the electron. However, its magnetic moment is around 600 times less than that of the electron.

### 1.10 The Electron Cloud

(Bauer 1922; Birtwistle 1926; Campbell 1924; Jouguet 1964, p. 24; Bessis 1978, p. 5; Filippi 1965, p. 245; Mahan et al. 1970, p. 409; Van de Vorst 1992, p. 23)

In 1913, Niels Bohr (1885-1962) (Lurçat 2001) proposed a coherent model that accounted for the various spectral lines measured experimentally, resulting in the enormous success of this model, also known as the Bohr-Sommerfeld model (Génie

Fig. 1.7 Thomson's atomic model (1907)


Infographie Margue $\dagger$

Fig. 1.8 The RutherfordPerrin atomic model (1911): negative electrons orbit around a positive nucleus

de la science n ${ }^{\circ} 34$ 2008). Bohr's theories were widely disseminated in France by Léon Brillouin (1889-1969), who in 1922 produced an astonishingly modern book on this question (Figs. 1.7 and 1.8) (Photo 1.11) (Brillouin 1922).

Bohr himself describes his atomic theory using the quantum postulate in (Bohr 1932). The electrons gravitate around the nucleus containing protons and neutrons. This model is universally held as the reference model today, although the view of stable deterministic orbits is somewhat misleading and a statistical approach is necessary to appreciate the reality of the electron shells. In his theory, Bohr sets out two key postulates:

- Electrons describe a circular orbit around the nucleus of the atom and conserve their energy. Consequently, they do not behave as predicted by classical mechanics and electrodynamics, namely that they should radiate (by emitting electromagnetic radiation) while moving around the nucleus, thereby losing energy, and falling towards the nucleus like a satellite falling back to Earth.


Photo 1.11 Niels Bohr, celebrated in a Danish stamp (left), and Léon Brillouin, a French pioneer of quantum physics (The Marguet collection and public domain)

As long as an electron moves around the same orbit, it conserves its energy and the orbital is said to be "stationary".

- The transition from one orbit (of quantified energy $E_{1}$ ) to another (of energy $E_{2}$ ) results in the emission (or absorption) of one photon of energy: $h \nu=\left|E_{1}-E_{2}\right|$

The forces applied to the electron must cancel each other out in order for the orbit to remain stable. The electron is subjected to centrifugal force and to the Coulombic force of attraction exerted by $Z$ protons in the nucleus:

$$
\frac{m v^{2}}{r}-\frac{1}{4 \pi \varepsilon_{0}} \frac{Z e^{2}}{r^{2}}=0
$$

Bohr next introduced a quantification hypothesis taking the stable circular orbit to be a whole multiple of the De Broglie wavelength associated with the electron:

$$
2 \pi r=n \lambda=n \frac{h}{m v}
$$

The quantity $h /(2 \pi)$, written as $\hbar$ (pronounced " $h$ bar"), constitutes the "quantum of action" introduced by Max Planck (1858-1947) in 1901 in his electromagnetic wave theory (Génie de la science, No 27 2006), in which the Planck constant $h$ is incorporated in the international MKS system ${ }^{14}$ :

$$
h \equiv 6.6260755 \times 10^{-34} \pm 6 \times 10^{-5} \% \text { J.s }
$$

The introduction of $h$ confers particle properties on waves also applicable to photons of frequency $\nu$, energy $E=h \nu$, speed in vacuum $c$ and relativistic mass $m=E / c^{2}$. Bohr's hypothesis thus supposes that the electron cloud is made up of a

[^10]number of electron shells, $K, L, M, N$, and so on. Within these shells, the trajectories and energy of electrons may be quantified. The orbits are considered to be practically circular with a radius $r$. The condition for quantification is that the stable orbit of an electron may only be a whole multiple ( $n$ ) of $\lambda$. The number $n$ is the first quantum number. This may be depicted visually as a string vibrating at wavelength $\lambda$ (which is thus the distance between two vibratory nodes), and which we may convert into a round loop or lasso having a circumference of $2 \pi r$. In order for the link to be stable, this length must be a whole multiple of the wavelength, i.e. $2 \pi r=n \lambda$ (the end of the lasso closing the loop must be a node). The condition for quantification thus requires that the kinetic moment be expressed as the whole product of the quantum of action $\hbar: m v r=n \hbar$ where $n$ is the principal quantum number and is a whole number equal to or greater than 1 . The two equations:
$$
2 \pi r=n \lambda=n \frac{h}{m v} \quad \text { and } \quad \frac{m v^{2}}{r}=\frac{1}{4 \pi \varepsilon_{0}} \frac{Z e^{2}}{r^{2}}
$$
give the radius of the stable orbits:
$$
r=\frac{n^{2}}{Z} \frac{h^{2} 4 \pi \varepsilon_{0}}{4 \pi^{2} m e^{2}}=\frac{n^{2}}{Z} \frac{h^{2} \varepsilon_{0}}{\pi m e^{2}} \text { and the speeds }: v=\frac{Z e^{2}}{2 n h \varepsilon_{0}} .
$$

In numerical terms, the calculation may be made for the hydrogen atom ${ }_{1}^{1} H$ as follows:

$$
Z=1, m_{e^{-}}=9.109534 \times 10^{-31} \mathrm{~kg}, h=6.6260755 \times 10^{-34} \mathrm{~J} . \mathrm{s},
$$

Vacuum permittivity:

$$
\varepsilon_{0}=\frac{1}{\mu_{0} c^{2}}=8.8542 \times 10^{-12} F . m^{-1}
$$

Vacuum permeability:

$$
\mu_{0}=4 \pi 10^{-7} H \cdot m^{-1}
$$

giving the value of the nearest radius $r_{1}=5.293 \times 10^{-11} \mathrm{~m}=0.53 \AA$ ㅇ where $n=1$ and $v=2200 \mathrm{~km} / \mathrm{s}$, i.e. $6.5 \times 10^{15}$ revolutions per second. This absolutely colossal figure gives an idea of the notion of the electron cloud. The electron configuration is represented in certain drawings as blurred orbits in which the electron itself is not depicted. The energy of the electron in its trajectory comprises the sum of its kinetic energy:

$$
E_{c}=\frac{1}{2} m v^{2}=\frac{1}{4 \pi \varepsilon_{0}} \frac{Z e^{2}}{2 r}
$$

and its potential energy, i.e the energy required to separate the electron entirely from the nucleus:

$$
E_{p o t}=\int_{r}^{\infty} f_{a}(r) d r=-\int_{r}^{\infty} \frac{1}{4 \pi \varepsilon_{0}} \frac{Z e^{2}}{r^{2}} d r=-\frac{1}{4 \pi \varepsilon_{0}} \frac{Z e^{2}}{r}
$$

Thus, the total energy of the electron in its trajectory corresponding to the principal quantum number $n$ for an atom of atomic number $Z$ is given by:

$$
E_{\text {total }}=E_{c}+E_{p o t}=\frac{Z e^{2}}{8 \pi \varepsilon_{0} r}-\frac{1}{4 \pi \varepsilon_{0}} \frac{Z e^{2}}{r}=-\frac{Z e^{2}}{8 \pi \varepsilon_{0} r}=-\frac{Z^{2}}{n^{2}} \frac{m e^{4}}{8 h^{2} \varepsilon_{0}^{2}}
$$

This same result may also be obtained by writing out the equation of Erwin Schrödinger (1887-1961) (Peaslee and Mueller 1955, p. 225), $H[\psi]=E \psi$ associated with the potential energy which is here reduced to the Coulombic energy of attraction. In this case, the Hamiltonian operator applies (Julg 1970, p. 23):

$$
H[]=\left(-\frac{h^{2}}{8 \pi^{2} m} \Delta-\frac{Z e^{2}}{r}\right)[]
$$

The most negative energy corresponding to the electron most strongly bound to the central nucleus is given for $n=1$ by the following:

$$
E_{1}=-\frac{Z^{2} m e^{4}}{8 h^{2} \varepsilon_{0}^{2}}
$$

The other stationary orbits are characterized by the energy levels $E_{n}=E_{1} / n^{2}$. The numerical value for hydrogen is $E_{1}=13.6 \mathrm{eV}$. Quasi-stationary orbits have the following energy (Duquesne et al. 1960, p. 12):

$$
E_{n}=\frac{E_{1}}{n^{2}}=-\frac{Z^{2} m e^{4}}{8 n^{2} h^{2} \varepsilon_{0}^{2}} \text { where } E_{1}=-13.6 \mathrm{eV}
$$

This energy corresponds to that of the photon emitted when a resting electron is bound to a proton to form a hydrogen atom (Berthelot 1956, p. 6; Hume-Rothery 1959, p. 72). The wavelength of the radiation emitted during transition between one orbit, $n_{1}$, and another, $n_{2}\left(n_{2}<n_{1}\right)$, is given by (Fig. 1.9):

$$
h \nu=h \stackrel{c}{\lambda}=\Delta E=E_{1}-E_{2}=\frac{Z^{2} m e^{4}}{8 n_{2}^{2} h^{2} \varepsilon_{0}^{2}}-\frac{Z^{2} m e^{4}}{8 n_{1}^{2} h^{2} \varepsilon_{0}^{2}}
$$

Bohr's theory was confirmed in practice by the experiments of James Franck (1882-1964) and Gustav Hertz (1887-1975), ${ }^{15}$ conducted as of 1911 and published

[^11]

Fig. 1.9 Bohr's model of the hydrogen atom (1913)
in 1914 (Born 1971, p. 100; Filippi 1965, p. 234; Rival 1996, p. 132). Both men were awarded the Nobel Prize for physics in 1925 for the discovery of the laws governing collision between electrons and atoms. In a tube filled with mercury vapor, electrons are accelerated using a variable electrical field. When the applied voltage is increased to 4.9 Volts, inelastic collisions occur and the electrons lose practically all of their kinetic energy (Fig. 1.10).

This value of 4.9 V is explained by the spectrum of mercury according to Bohr's theory, and generalization of this method enables precise measurements to be made of the different series of spectral lines of hydrogen giving the series of J.J. Balmer (1825-1898) (around $\lambda=5000 \AA_{A}^{\circ}$ in the visible range, (Jouguet 1964, p. 23)) and

[^12]

Fig. 1.10 Series of spectral lines emitted by the hydrogen atom
T. Lyman (1874-1954) ( $\lambda \approx 1000 \AA$ A ) in the ultraviolet, and of F. Paschen (1865-1947) and F.S. Brackett (1896-1988) in the infrared. An electron having positive energy is no longer restricted to orbiting around the nucleus and is referred to as a free electron, the ordered movement of which creates an electrical current. For positive energies, there is no more quantification, and here we are back in the territory of classical electromagnetic theory. The energy of the non-relativistic electron is given by its kinetic energy:

$$
E=\frac{1}{2} m v^{2}
$$

The wavelength of de-excitation emissions by the photon is given by the formula:

$$
\frac{1}{\lambda}=\frac{Z^{2} m e^{4}}{8 h^{3} c \varepsilon_{0}^{2}}\left(\frac{1}{n_{2}^{2}}-\frac{1}{n_{1}^{2}}\right)
$$

As applied to hydrogen, the empirical formula (1888) of Johannes Rydberg (1854-1919) and Walther Ritz (1878-1909) is as follows:

$$
\begin{equation*}
\text { the Rydberg-Ritz formula: } \frac{1}{\lambda}=\frac{m e^{4}}{8 h^{3} c \varepsilon_{0}^{2}}\left(\frac{1}{n_{2}^{2}}-\frac{1}{n_{1}^{2}}\right) \tag{1.2}
\end{equation*}
$$

where $R_{H} \equiv \frac{m e^{4}}{8 h^{3} c \varepsilon_{0}^{2}}=1.09737315 \times 10^{7} \mathrm{~m}^{-1}$ is the Rydberg constant, occasionally written as $R_{\infty}$.

$$
h c R_{H}=13.606 \mathrm{eV}=1 R y .
$$

More accurately, it must be remembered that the photon is generated with an impulse of $E_{\gamma} / c$. Thus, conservation of the total impulse before emission (at which point it is nil since the atom is immobile within the referential associated with it) and after emission, indicates that the emitting atom is also subjected to a recoil impulse nominally equivalent to that of the photon. In fact, the energy carried away by the photon is very slightly weaker than that predicted by Bohr's theory. It should nevertheless be noted that quantification of the energy levels (phonons) within a crystal allows for the emission of a photon without recoil of the emitting nucleus (the Mössbauer (1929-2011) effect (Photo 1.12), discovered in 1957 by analysis of $\gamma$ emission at 129 keV by iridium 191, for which the recoil energy of the free atom is $0.05 \mathrm{eV})$. The recoil energy is thus transferred to the entire crystal lattice rather than to the target atom and results in Doppler broadening (Seidel 1967, p. 1). Indeed, following an impulse of $E_{\gamma} / c$, an emitting nucleus possesses a certain degree of quantum recovery while the state of the lattice remains unchanged.

The inverse phenomenon (recoil-free collision with a photon) is also possible (Born 1971, p. 247; Cohen-Tannoudji et al. 1988, p. 494). The practical use of this effect is the production of perfectly monochromatic photons for physics and chemistry experiments requiring great precision (Mössbauer spectroscopy using $\gamma$ fluorescence by nuclear resonance). When the spectral lines for hydrogen are observed with an extremely precise spectrometer, a macroscopic line is seen to comprise several very close adjacent lines. Arnold Sommerfeld (1868-1961) developed Bohr's theoretical calculus, proposing elliptical rather than circular orbits for electrons (Duquesne et al. 1960, p. 13; Jouguet 1964, p. 34; White

Photo 1.12 Rudolph
Ludwig Mossbauer, awarded the Nobel Prize for Physics in 1961 for the discovery of the effect that bears his name (Public domain)


1934, p. 42). The total energy is given by $E=-Z e^{2} /(2 a)$ where $a$ is the semi-major axis of the ellipse (Bayet 1960, p. 75). The energy is thus given by the following formula using a second quantum number, $l$, known as the orbital quantum number:

$$
E_{n, l}=-\frac{2 \pi^{2} Z^{2} m e^{4}}{n^{2} h^{2}}\left(1+\frac{\alpha^{2} Z^{2}}{n^{2}}\left(\frac{n}{l+1}-\frac{3}{4}\right)\right)
$$

where $\alpha_{[-]}=\frac{e^{2}}{2 \varepsilon_{0} h c}=\frac{1}{137.04}$ is the fine-structure constant
In particular, Sommerfeld's theory provides an explanation of the effect discovered in 1896 by Pieter Zeeman (Jouguet 1964, p. 70; Filippi 1965, p. 176; White 1934, p. 149), in which spectral lines split up into a variable number of components under the effect of a magnetic field (Renault 1948, p. 77; Herzberg 1991, p. 103; Condon and Shortley 1959, p. 378). The normal Zeeman effect describes the splitting of a spectral line of frequency $\nu_{0}$ into three separate components under the effect of a magnetic field $B$ : the non-displaced line and two lines of frequency $\nu=\nu_{0} \pm e B /(4 \pi m)$. Sommerfeld also used the laws of relativity, which hold that the mass of an electron increases with its speed, and this effect must not be neglected for certain electron shells. All of these improvements allowed an explanation to be given for this phenomenon of extremely close spectral lines which together form a single mean line. Since then, physicists refer to the Bohr-Sommerfeld model. However, the Bohr model deviates from the experimental measurements as the value of $Z$ increases and recourse to wave mechanics becomes necessary. More precisely, the energy state of an atom (i.e. of its electrons) is entirely determined by a wave function, the solution to the Schrödinger equation, which involves the use of four quantum numbers (Born 1971, p. 115):
$n$ the principal quantum number, which has values of $1,2,3$, etc., and defines the electron shells $K, L, M$, and so on; this number is associated with the total energy of the electron. Each shell may contain up to $2 n^{2}$ electrons.
$l$ the orbital or azimuthal quantum number, also occasionally referred to as the quantum number of angular moment, which has integer values of 0,1 , etc., $n-1$ and defines for shell $n$ the respective sub-shells $s, p, d, f$, and thus the eccentricity of the orbital. A pair of values $(n, l)$ defines an electron shell. Orbiting electrons create intra-atomic currents that give rise to a magnetic moment (Jouguet 1964, p. 40). If an electron has an angular moment, it has kinetic energy of angular movement, which is naturally limited by the overall quantity of energy, as quantified by $n . l$ is thus logically limited by $n$ (Mahan et al. 1970, p. 423).
$m$ the magnetic quantum number: $m=-l,-(l-1) \ldots,-1,0,1, \ldots, l-1, l$. A set of values $(n, l, m)$ defines a quantum state. $m$ defines the spatial orientation of the orbital of the electron, i.e. the projection on a given axis of the moment of the quantity of movement of the electron, which may be $m \hbar$ for the different values of $m$. These quantifiable values may only be detected under the effect of an external magnetic field. $m$ may only take $2 l+l$ values (Fig. 1.11). It is


Fig. 1.11 Depiction of the quantification of orbital moment in a magnetic field
the electrons moving within the atom that create intra-atomic currents which give rise to a magnetic moment. Since this moment originates in the angular moment, it is naturally limited by the value of $l$.
$s$ the spin quantum number: the hypothesis of the electron spinning around its own axis and behaving like a small magnet was put forward in 1925 by G. Uhlenbeck (1900-1988) and S. Goudsmit (1902-1978) (Bayet 1960, p. 789; Filippi 1965, p. 253). This spin or intrinsic moment of the electron may only take one of two values: $+1 / 2$ or $-1 / 2$ in $\hbar$ units. It characterizes a kinetic moment specific to the particle which may be said to be "spinning about itself". ${ }^{16}$ The famous experiment conducted in 1922 by O. Stern (1888-1969) and W. Gerlach (1889-1979) showed (Cagnac and PebayPeyroula 1995, p. 235; Herzberg 1991, p. 193; Jouguet 1964, p. 68; Filippi 1965, p. 255) that the projection of the spin of an electron in the direction of an external magnetic field could have only two values (parallel or antiparallel) (Born 1971, p. 169), (Duquesne et al. 1960, p. 13). The spin of an electron is thus either $\hbar / 2$ or $-\hbar / 2$.

In 1924 (De Maria 2002, pp. 38-39), Enrico Fermi published an article in the famous Italian physics journal Nuovo Cimento on statistical mechanics entitled "Considerations on the quantification of systems containing identical elements". ${ }^{17}$ Indeed, Fermi had been working since 1923 on quantifying the states of molecules of an ideal gas which move around without friction while exchanging energy on each collision with other molecules. Furthermore, in December 1923, he published an article in the Rendiconti dell'Accademia Nazionale dei Lincei, entitled "On

[^13]Stern's Theory of the Absolute Constancy of the Entropy of a Perfect Monoatomic Gas", ${ }^{18}$ in which he demonstrated that there is no need for the zero-point molecular energy hypothesis proposed by Otto Stern (1888-1969) in order to establish the entropy of a monoatomic ideal gas as calculated by the German physicists Otto Sackur (1880-1914) and, independently, Hugo Tetrode (1895-1931). In the second article published in 1924, Fermi concerned himself with the inability of the BohrSommerfeld model to describe the spectral lines of atoms heavier than hydrogen. Citing Fermi, De Maria explained that: "Such failure is genuinely attributed to the fact that these more complex systems do not allow the separation of variables ${ }^{19} \ldots$ In this study, I intend to show that this failure seems rather to be due to the inadequate conditions under which Sommerfeld calculated the statistical orbitals of systems possessing identical elements". In the example of the helium atom, the two electrons orbiting around a nucleus cannot be distinguished on the sole basis of their quantum numbers. Fermi thus modified the conditions for quantification of ideal gases containing identical molecules, namely that each of the elementary cells into which the volume of gas is discretized may contain only one molecule. Fermi deduced by an unjustified reasoning that Sommerfeld's conditions of quantification were not applicable to an atom containing identical subatomic elements (in this case, electrons). It was the Austrian physician Wolfgang Pauli who, in January 1925, discovered what is known today as the Pauli exclusion principle. On reading Pauli's article, Fermi realized that he could complete his theory of an ideal gas obeying the so-called Fermi-Dirac statistics, since in 1926 Paul Dirac would attain the same results as Fermi using a different approach.

The exclusion principle of Wolfgang Pauli (1900-1958) postulated in 1924 states that no two electrons can have the same set of quantum numbers (Born 1971, p. 162; Herzberg 1991, p. 121; Foderaro 1971, p. 241). Only one electron is permitted for each state. Although not the result of any tried and tested theory, this principle accurately describes the way in which the electron shells are constructed (Photo 1.13).

The magnetic moments $\vec{l}$ and $\vec{s}$ are composed in vectorial fashion (Herzberg 1991, p. 187) so that two results may be obtained: either $j=l+1 / 2$ or $j=l-\frac{1}{2}$. For each value of $l$, there is thus a corresponding derived internal quantum number known as $j$. The quantum levels of an atom are filled with electrons successively in accordance with a few simple rules, clarified by experience: each orbital has a corresponding energy level (an energy previously calculated very precisely), and the electrons are always added in such a way that this energy remains as low as possible, but according to the Pauli exclusion principle, no two electrons in the same atom may have the same four quantum numbers. Finally, Hund's rules apply (Julg 1970, p. 31; Mazenko 2000, p. 361) and these are two-fold: first, within the same energy level, all locations in one orbital must contain an electron before filling

[^14]

Photo 1.13 Wolfgang Ernst Pauli (1900-1958). A child prodigy in mathematics, he was the stepson of the renowned physician Ernst Mach, after whom he was given his middle name. Following his studies at the University of Munich, where he was taught by Arnold Sommerfeld, at the request of his master, he drew up at the age of 21 years a synthesis of special relativity for the five-volume Encyclopaedia of Mathematics in German. He obtained his doctorate in 1921 for his thesis dealing with the hydrogen atom in which he demonstrated the limitations of Bohr's quantification rule. He taught in Zurich but left in 1935 to teach in the United States, where he spent the war years. He returned to Switzerland after the war and was involved in the creation of the CERN. He was awarded the Nobel Prize in physics in 1945 for his discovery of the exclusion principle that bears his name (Public domain)
is completed by the formation of pairs having opposite spin; second, in the most stable state, electrons occupy the highest possible number of orbitals of the same type: for instance, carbon has two $2 p$ orbitals while nitrogen has three. In oxygen, which contains four $2 p$ electrons, one orbital is doubly occupied and two are singly occupied. Regarding photon emission, the only transitions between two quantum states allowed are those for which:

$$
l_{\text {final }}-l_{\text {initial }}= \pm 1, s_{\text {final }}-s_{\text {initial }}=0, j_{\text {final }}-j_{\text {initial }}= \pm 1
$$

one level may thus contain a maximum of $2 \sum_{l=0}^{l=n-1}(2 l+1)=2 n^{2}$ electrons. Each level is associated with $n^{2}$ orbitals, i.e. $2 n^{2}$ Schrödinger wave functions, taking spin into account (Table 1.2).

| $\mathrm{K}(n=1)$ | 2 electrons | 2 s | $(l=0)$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{L}(n=2)$ | 8 electrons | 2 s | $(l=0)$ |
|  |  | 6 p | $(l=1)$ where $m=-1,0,+1$ |
| $\mathrm{M}(n=3)$ | 18 electrons | 2 s | $(l=0)$ |
|  |  | 6 p | $(l=1)$ |
|  |  | 10 d | $(l=2)$ where $m=-2,-1,0,1,2$ |


| $\mathrm{N}(n=4)$ | 32 electrons | 2 s | $(l=0)$ |
| :--- | :--- | :--- | :--- |
|  |  | 6 p | $(l=1)$ |
|  |  | 10 d | $(l=2)$ |
|  |  | 14 f | $(l=3)$ where $m=-3,-2,-1,0,1,2,3$ |

Table 1.2 Distribution of orbitals in electron shells

| $n$ | $s$ | $p$ | $d$ | $f$ | $\ldots$ |
| :--- | :--- | :--- | :--- | :--- | :---: |
| 1 | 2 |  |  |  | $\vdots$ |
| 2 | 2 | 6 |  |  | $\vdots$ |
| 3 | 2 | 6 | 10 |  | $\vdots$ |
| 4 | 2 | 6 | 10 | 14 | $\vdots$ |
| $\vdots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\vdots$ |

Let us take as an example chlorine, which has 17 electrons $(Z=17)$. The first electrons fit in the $K$ shell, which has the lowest energy and accepts a maximum of 2 electrons. We label them $1 \mathrm{~s}^{2}$, indicating that there are 2 electrons in sub-shells $(l=0)$ of the $K$ shell $(n=1)$. The following electrons fit into the L shell $(n=2)$; first, 2 electrons in sub-shells $(l=0)$, then 6 electrons in sub-shell $\mathrm{p}(l=1)$, $[m=-1,0,+1]$. These are followed by the last 7 electrons ( $2 \mathrm{~s}, 5 \mathrm{p}$ ). Bohr's planetary electron model should not allow us to overlook the fact that the atom is essentially empty. If the nucleus of a hydrogen atom were represented as a quarter coin, at scale, its electron would be orbiting at about 1 km from the coin! The standard representation of the electron cloud which, for obvious reasons of space, is drawn next to the nucleus, tends to mask this reality. The origin of the spontaneous emission that results in an electron passing from a far orbit to a closer orbit is in fact vacuum fluctuation. Such fluctuation is due to so-called zero-point energy in the quantum vacuum state. The quantum vacuum state is the final phase that subsists after a material vacuum has been created in an empty box (i.e. removal of the slightest atom of matter from the space using a perfect vacuum pump). At this level of a classical vacuum, thermal radiation subsists due to the temperature of the walls of the box. If the walls of the container are cooled to 0 kelvin, irreducible non-thermal electromagnetic radiation subsists at the zero point, the effects of which have been demonstrated by Willis Lamb (1913-2006) and by Hendrik Casimir (1909-2000).

### 1.11 The Atomic Nucleus

(Barret and Jackson 1977; Evans 1955; Held 1991; Mayo 1998; Savushkin and Toki 2004; Trocheris 1959; Nuclear Structure 1960)

Experimentally, the rest mass of the nucleus is lower than the rest mass of its constituents when they are free, namely protons $(Z)$ and neutrons $(A-Z)$ :

$$
M_{Z} X<Z m_{1 p}+(A-Z) m_{0^{1} n}+Z m_{-1}^{0} e^{-}
$$

Enrico Fermi (1901-1954) proposed an empirical formula for the mass of isotopes (Soodak 1955) that collates well with the experimental values:

$$
M_{Z}^{A} X \approx 1.01464 A+0.014 A^{\frac{3}{2}}-0.041905\left[C_{A}+\frac{\left(Z-C_{A}\right)^{2}}{C_{A}}\right]+\lambda \frac{0.036}{A^{\frac{3}{4}}}
$$

where: $\left\{\begin{array}{ll}\lambda=+1 & \text { when } A \text { is even, } Z \text { is odd } \\ \lambda=-1 & \text { when } A \text { is even, } Z \text { is even } \\ \lambda=0 & \text { when } A \text { is even, irrespective of } Z\end{array}\right.$ and

$$
C_{A}=\frac{A}{1.98067+0.0149624 A^{\frac{3}{2}}}
$$

This mass defect (defined in positive form) is given by (Jouguet 1964, p. 214):

$$
\Delta m=Z m_{1} p+(A-Z) m_{0^{1} n}+Z m_{-0}^{0} e^{-}-M_{Z} X
$$

The mass defect may be expressed as energy (using the Einstein formula) and corresponds to the binding energy released on formation of the nucleus from protons and neutrons. The binding energy may thus be calculated from the mass defect. Taking $1 \mathrm{u}=931.54 \mathrm{MeV} / \mathrm{c}^{2}$, we obtain the following relationship (Table 1.3):

$$
E_{\text {binding }[\mathrm{MeV}]}=931.54_{[\mathrm{MeV} / \mathrm{u}]} \Delta m_{[u]}
$$

The curve of Aston (Fig. 1.12), who, beginning in 1920, had measured with great precision the different mass defects (Born 1971, p. 69), plots the variation in binding energy per nucleon $E_{\text {binding }} / A$ in $\mathrm{MeV} /$ nucleon as a function of the number of nucleons $A$.

This curve presents irregularities particularly visible at low mass numbers corresponding to highly stable isotopes such as ${ }_{2}^{4} \mathrm{He}$ with high binding energy per nucleon. These "magic" numbers of nucleons are explained by the closed shell model of the nucleus, as we shall see below. Fission involves displacing the right-

Table 1.3 Binding energy of three selected isotopes

|  | Atomic <br> mass $(\mathrm{u})$ | Mass of <br> neutrons <br> $(\mathrm{u})$ | Mass of <br> protons <br> $(\mathrm{u})$ | Mass of <br> electrons <br> $(\mathrm{u})$ | Mass <br> defect <br> $(\mathrm{u})$ | Binding energy per <br> nucleon <br> $(\mathrm{MeV} /$ nucleon $)$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| ${ }_{92}^{235} \mathrm{U}$ | 235.044 | 144.009 | 92.672 | 0.050 | 1.914 | 7.592 |
| ${ }_{51}^{132} \mathrm{Sb}$ | 131.885 | 81.729 | 51.371 | 0.028 | 1.216 | 8.581 |
| ${ }_{41}^{101} \mathrm{Nb}$ | 100.911 | 60.520 | 41.298 | 0.022 | 0.930 | 8.575 |



Fig. 1.12 Aston's curve: binding energy per nucleon as a function of mass number A


Photo 1.14 Francis William Aston (1877-1945), official photo for the Nobel Prize for Chemistry in 1922 (Public domain)
hand section of Aston's curve (for a heavy fissile isotope like uranium 235) towards the center, and thus increasing the binding energy per nucleon (Photo 1.14).

Fusion consists of displacing the left-hand part of Aston's curve, again towards the center. The increase in binding energy corresponds to the provision of available energy. The binding energy is the mean energy lost by each nucleon in the formation of the nucleus in question. If, on the contrary, we wish to tear away a nucleon from the nucleus, we must supply a mean quantity of energy equal to the binding energy per nucleon. In practice, the binding energy of a given nucleon is not strictly equal to the mean binding energy per nucleon, but depends on the nucleon shell in which the nucleus is found.

The binding energy per nucleon is one of the criteria for stability of a nucleus. Beyond a certain high mass number, all nuclei become fissile. Francis William Aston, who was Joseph John Thomson's assistant around 1910, invented the mass spectrometer (he was awarded the Nobel Prize for chemistry in 1922): the impact on a photographic plate of ions deflected in an electromagnetic field leaves tracks that may be calculated by means of parabolic ballistic analysis. This method allows precise measurement of the mass of ions and of atoms.

The precision of Aston's mass spectrometer enabled him to carry out experiments to determine the mass defect (also known as packing fraction) resulting in the intra-atomic binding energy plotted on the curve. Not all combinations of $Z$ protons and $A-Z$ neutrons are intrinsically stable. Only some 280 nuclei are stable, with the other naturally occurring nuclei disappearing over time in accordance with an immutable law independent of external conditions: such nuclei are said to be radioactive and to disintegrate. This disintegration is frequently accompanied by the emission of photons of energy having zero mass. Very "heavy" nuclei are unstable. Today, super-heavy nuclei may be created artificially in an accelerator, and the magic numbers theory predicts an island of stability at around $Z=114$, which we are gradually approaching. At this weight level, the stability of a substance simply indicates an exceptionally long life in comparison with its neighbors of similar $Z$ values. Experiments show that the density of nuclear matter made up of nucleons (protons and neutrons) is relatively constant:

$$
\frac{A}{\frac{4}{3} \pi R^{3}} \approx \text { constant hence } R=R_{0} A^{1 / 3} \text { where } R_{0}=1.28 \pm 0.05 \mathrm{fm}
$$

It has been experimentally demonstrated that the constant $R_{0}$ is higher for light nuclei $(\cong 1.3)$ than for heavy nuclei $(\cong 1.3)$. Closer analysis of the nucleus shows that the nuclear density is not entirely constant within a sphere of radius $R$ but follows the empirical law of so-called Fermi distribution (Barret and Jackson 1977, p. 8; Foderaro 1971, p. 216; Nuclear structure 1960, p. 25; Valentin 1982a, b, p. 25), which takes the following form (Fig. 1.13):

$$
\rho(r) \approx \frac{\rho_{0}}{1+e^{\frac{r-R}{0.228} e}} \text { where } e \text { is the "skin" thickness } \approx 2 \mathrm{fm}
$$

This form is used in the optic model of elastic diffusion in the context of the Woods-Saxon refraction potential, established in 1954, which takes the form $-V_{0} \rho(r)=-V_{0} /\left(1+e^{\frac{r-R}{e}}\right)$, and for which Schrödinger's equation can be solved (Foderaro 1971, p. 369). The cohesion of the nucleus, which is concentrated in a pseudo-sphere of radius $R$, is ensured by nuclear forces which compensate for the Coulomb (electrostatic) repulsive force between charged protons $+e$ (charges with opposite signs attract, while charges with similar signs repel one another).The strong interaction, which explains the strong bond between nucleons within the nucleus (i.e. why positively charged protons do not repel one another), is associated


Fig. 1.13 Nuclear density as a function of radius
with the existence of the meson, a heavy particle predicted in 1935 by Japanese physicist Hideki Yukawa ${ }^{20}$ (1907-1981) (Dodd 1984, p. 46; Mathieu 1991, p. 231), and discovered in 1936 (meson $\mu^{ \pm}$by Carl D. Anderson (1905-1991) and Seth H. Neddermeyer (1907-1988)), then in 1946 (meson $\pi^{ \pm}$by Cecil F. Powell (1903-1969)). The strong interaction is an extremely powerful force $\left(10^{+39}\right.$ times greater than gravity, 100-1000 times stronger than electromagnetic forces!), but is exerted over a very short distance of several fm. The quantum of action of this strong force, the $\pi$ meson or pion, has a mass of $137 \mathrm{MeV} / \mathrm{c}^{2}$. The nucleons of a single nucleus continually exchange mesons depending on their configuration. The proton-neutron interaction having as its mediating particle a meson $\pi^{+}$is expressed as:

$$
\text { Interaction } p-n:{ }_{1}^{1} p+{ }_{0}^{1} n \rightarrow{ }_{o}^{1} n^{\prime}+\pi^{+}+{ }_{0}^{1} n \rightarrow{ }_{o}^{1} n^{\prime}+{ }_{1}^{1} p^{\prime}
$$

The weak interaction, which acts on both hadrons and leptons, is $10^{5}$ times weaker than the strong interaction (GA Vol. 1 1967, p. 49; Valentin 1982a, b, p. 89), and operates over a distance of less than $10^{-18} \mathrm{~m}$ (Dodd 1984, p. 34). It allows explanation of $\beta$ radioactivity, and Enrico Fermi, in his theoretical masterpiece for which he won the Nobel Prize for physics in 1938, posited in late 1933 a complete theory of $\beta^{-}$disintegration (Dodd 1984, p. 66). This theory is based upon Pauli's proposition of a light neutral entity (in Italian, "neutrino" = small neutron, as opposed to "neutrone", i.e. James Chadwick's neutron), and accounts for why electrons from $\beta^{-}$disintegration have a continuous emission spectrum, while the initial and final states of the electron are completely quantified. Indeed, energy is carried away by the neutrino at the same time as electron emission. The mediating particle of weak interaction is the boson. On analysis of the stability of nuclei, greater stability is seen for nuclei comprising $8,20,50,82$ or 126 neutrons or

[^15]protons. Oxygen 16 (with 8 neutrons and 8 protons), calcium 40 (with 20 neutrons and 20 protons), zirconium 90 (with 40 protons and 50 neutrons), cerium 140 (with 82 neutrons and 58 protons) and lead 208 (with 126 neutrons and 82 protons) are experimentally highly stable. This stability is immediately reminiscent of the high degree of chemical stability of those elements containing a filled outer electron shell (the rare gases), which gave rise to the idea of a shell model of nucleons (Born 1971, p. 279). It was Eugen P. Wigner (1902-1995) who described these isotopes as magic, and this remains the standard term. James H. Bartlett (1904-2000), Kurt Guggenheimer and Walter Elsasser (1904-1991) immediately proposed a model of individual particles in closed shells containing $2(2 l+1)$ neutrons or protons per shell ( $l$ : quantum number of the angular moment or orbital). However, this model only explained the magic numbers up to ${ }_{8}^{16} O$ (i.e. until the first $p$ orbital has been filled).

It was in fact studies by Maria Goeppert-Mayer ${ }^{21}$ (1906-1972) from 1948 onwards that proved the existence of shells for nucleons of the same type (protons or neutrons) of 50, 82 and 126 (Lilley 2001, p. 45). The term "magic numbers" was

[^16]
(The Marguet collection)


Fig. 1.14 The electrostatic potential energy barrier within the nucleus
introduced. By invoking intense spin-orbit ${ }^{22}$ coupling forces (" $j$ - $j$ coupling") based on an idea of Enrico Fermi ("might there be a spin-orbit coupling index?"), she discovered the magic numbers. Hans Jensen (1907-1973) developed a parallel theory, and he and Maria Mayer jointly shared the Nobel Prize for physics in 1963 (with the other share going to Eugen Wigner for his work on the interactions between nucleons). However, Maria Mayer's theory does not explain everything since extremely heavy isotopes like chemical bodies (such as lithium 11!) appear to have been discovered, and these could have the forms of "water molecules", which cannot be accounted for in the shell model.

According to electromagnetic field theory, a charged particle of atomic number $z$ experiences a Coulomb barrier (Fig. 1.14) of height $Z z e^{2} / R$ as the particle approaches a nucleus of charge $Z$. The nucleus sits in the potential well comprising nucleons characterized by four quantum numbers, as for electrons:

- the principal quantum number

```
n(>0)
\(l \leq n-1\) \(m \leq l-1\) \(s\)
```

- the orbital quantum number
- the magnetic quantum number
- the spin quantum number

The Wolfgang Pauli exclusion principle applies again as for electrons: two nucleons of the same type ( ${ }_{1}^{1} p$ or ${ }_{0}^{1} n$ ) cannot have identical quadruplets ( $n, l$, $m, s)$. The energetic well contains quantum levels in which protons and neutrons are held, starting with the lowest energy levels, according to Pauli's principle, thus dictating the maximum number of nucleons that provide strong stability (Table 1.4):

The phenomenon in question is identical to the filling of electron shells seen earlier as for the rare gases, which are extremely chemically stable. Figure 1.15 depicts the potential well of nuclear forces in the form of a rectangle. This well is

[^17]Table 1.4 Magic numbers of filled nucleon shells

|  |  | Total |
| :--- | :---: | :---: |
| 1st shell | 2 | 2 |
| 2nd shell | 6 | 8 |
| 3rd shell | 12 | 20 |
| 4th shell | 30 | 50 |
| 5th shell | 32 | 82 |
| 6th shell | 44 | 126 |



Fig. 1.15 Nuclear shell model
inherently deep (strong forces) and narrow (very small range of action), in contrast with the electromagnetic potential well (Coulomb barrier to the right with an infinite range of action).

In the ground state, i.e. at the lowest total energy level, if shells are represented as energy levels, the nucleons occupy the lowest shells. If excitation energy is applied to the nucleus, it is distributed between the various nucleons which are rearranged within the various shells above the ground state to create an excited nucleus. If energy is concentrated in a nucleon (which is of very low probability compared with distribution between all nucleons), it may reach a virtual level sufficient to overcome the barrier, in which case it will be emitted (Littler and Raffle 1957, p. 19). The associated states have insufficient energy to enable de-excitation. However, the virtual states, even below the barrier, allow the emission of a nuclear particle by means of a tunnel effect or tunneling. This effect depends on the wave function of the particle within the nuclear force field, which
determines whether the particle can be ejected from the nucleus or not. The shell model accounts for $\gamma$ radioactivity and stable nuclei at magic numbers. However, though it explains nuclear stability well, it provides a poor explanation of the dynamic behavior of heavy nuclei. In the liquid-drop model proposed in 1939 by Niels Bohr and John Wheeler (1911-2008), the nucleus is likened to a drop of incompressible material, whose density does not depend on the size of the nucleus. Within this drop, nucleons can move around in the same way as molecules inside a sphere. This model provides an explanation for the fission of heavy nuclei: on being struck by a neutron, the heavy nucleus is deformed like a drop of water on receiving a shock, before being split in two and achieving a stable form in relation to the principle of minimization of total energy (in this case two spheres). The liquid-drop model led to a theoretical expression of mass defect. The semi-empirical model posited by Carl F. Von Weizsäcker (1912-2007) suggested in 1935 that mass defect corresponding to the binding energy $E_{\text {binding }}$ be expressed as follows:

$$
\begin{gather*}
\text { Weizä cker's Formula (1935): } \Delta m=\frac{E_{\text {Binding }}}{c^{2}} \\
=a_{V} A-a_{S} A^{2 / 3}-a_{a} \frac{(A-2 Z)^{2}}{A}-a_{c} \frac{Z(Z-1)}{A^{1 / 3}}+\delta a_{p} \frac{1}{A^{3 / 4}} \tag{1.3}
\end{gather*}
$$

The various terms have an analogous meaning in fluid mechanics (Glasstone and Edlund 1972, p. 12; Kahan 1963, p. 86; Lilley 2001, p. 38; Mayo 1998, p. 55):
$+a_{V} A$ is an energy of volume $a_{V} \approx 14 \mathrm{MeV}$. It is an attractive energy proportional to the numbers of nucleons characterizing the fact that each nucleon is attracted by its neighboring nucleons.
$-a_{S} A^{2 / 3}$ is a term corresponding to a surface energy ( $A^{1 / 3}$ is proportional to the radius of the atomic nucleus), $a_{s} \approx 13 \mathrm{MeV}$. Indeed, nucleons near the nuclear surface are less strongly bound than those located "deep down". The energy of attraction is thus overestimated by a quantity proportional to the area as a result of a surface tension effect.
$-a_{a} \frac{(A-2 Z)^{2}}{A}$ is a term expressing symmetry energy and reflects the fact that the excess of neutrons decreases the total nuclear energy, $a_{a} \approx 19.5 \mathrm{MeV}$. This term refers to supernumerary neutrons in relation to protons, particularly in heavy nuclei. This excess is essential for a certain stability, so that the forces of nucleon attraction (strong interaction) are able to counteract the Coulombic force of repulsion that would be too strong in the event of supernumerary protons. Nevertheless, an excessively high number of neutrons reduces the binding energy.
$-a_{c} \frac{Z(Z-1)}{A^{1 / 3}}$ designates the Coulombic force of repulsion of protons, $a_{c} \approx 0.585$
MeV .
$+\delta a_{p} \frac{1}{A^{3 / 4}}$ is a term that allows us to take into account the relative stability of eveneven isotopes where: $\delta=1$ for even $Z$ and $N$ and $a_{p} \approx 33 \mathrm{MeV}, \delta=-1$ for uneven $Z$ and $N, \delta=0$ for uneven $A$ (even $Z$ and uneven $N$ or uneven $Z$ and even $N$ ).

Weizsäcker's formula yields a characteristic parabolic curve on tracing the binding energy for isobaric isotopes. The most stable nuclei are those presenting maximum binding energy, which can be calculated mathematically by derivation in relation to $Z$ ( $A$ constant). It should be noted that there is no single set of values for coefficient $a$ corresponding to all isotopes, and that the proposed values are in fact experimental compromises. Attempts were obviously made subsequently to unify these models by virtue of a so-called collective model (studies by Aage Bohr and B. R. Mottelson (Bohr and Broglia 1977; Mathieu 1991, p. 240), in which a central part of the nucleus is represented as a drop of liquid with the outer regions containing nucleons having their own excitation energy, somewhat like peripheral electrons. When the spherical nucleus is deformed, the grouping together of the orbits of nucleons in separate shells seems to disappear, allowing more uniform distribution. V. M. Strutinsky demonstrated the re-emergence of shells for non-nil but pseudo-periodic deformations. This results in pseudo-magic of certain nuclei that are naturally deformed in their rest state. In 1966, Strutinsky introduced a number of corrections into the liquid-drop model to take into account the shell structure. In this model, the fission barrier has two extremes (double-humped barrier) allowing a shape isomer state (Fig. 1.16).

A number of quantum states are found in the potential well of the ground state and in the shape isomer state. An isomer may emit a photon and undergo de-excitation to the ground state, but it may also fission if the incident neutron can provide the required excitation energy. This non-symmetric double hump accounts in particular for the asymmetric fragmentation of heavy nuclei seen in fission yield curves. Strutinsky's theory continues to be pertinent until scission of the nucleus. Indeed, while around $80 \%$ of the energy is distributed between the fission fragments, the remainder is found in the form of deformation and excitation


Fig. 1.16 Strutinsky's fission barrier model
energy, making certain fission products highly unstable with almost instantaneous emission of neutrons and photons. In rare cases of so-called cold fission, the fragments recover $100 \%$ of the fission energy. For an improved understanding of the nucleus and fission thereof, we must look to the so-called microscopic theories describing the movement of each nucleon in quantum interaction with its neighbors. The Hartree-Fock mean field theory (Douglas R. Hartree [1897-1958] and Vladimir A. Fock [1896-1974]) to determine the wave function and the energy of a quantum many-body system in a stationary state, and the Hartree-FockBogolyubov method (N.N. Bogolyubov [1909-1992]), which takes into account nucleon pairing, require enormous computer power since the determination of wave functions for $N$ nucleons is notoriously demanding in terms of calculation times. ${ }^{23}$

### 1.12 Nuclear Spin

Spin refers to the rotational movement of a particle (resp. nucleus) around itself. Along with spin, the angular moment of spin must be considered. Similarly, from orbital movement (for an electron for instance), an orbital angular moment may be determined. The total angular moment is the sum of the spin angular moment and the orbital angular moment. The nuclear angular moment is measured in units of $\hbar=h / 2 \pi$, as for the angular moment of electrons, protons and neutrons (which is in fact $\hbar / 2$ for these three particles). Neutron spin is said to be $1 / 2$. In general for nuclei, the angular moment is $\sqrt{I(I+1)} \hbar$ where $I$ is the quantum number of the nuclear angular moment, also referred to as nuclear spin. This spin is a whole number $(0,1$, 2 , etc.) for isotopes with an even mass number, but maybe a half number $(1 / 2,3 / 2,5 / 2, \ldots$ up to $11 / 2$ ) in other cases. At their fundamental level, even-even isotopes always have zero spin (0), while uneven-uneven isotopes have whole spin, and others have halfwhole spin. Quite logically, the nuclear angular moment of a nucleus is a combination of the angular moment of its components. The angular spin moment of a nucleus is a vector and is designated by $\vec{s}_{i}$, with an orbital angular moment being denoted as $\vec{I}_{i}$. The rules for combination are as follows:

- in the event of weak coupling, or Saunders-Russell coupling (Frederick A. Saunders[1875-1963] and Henry N. Russell[1877-1957]) (Herzberg 1991, p. 128; Condon and Shortley 1959, p. 187), the spin and orbital angular moments are added together and the nuclear spin angular moment is given by the sum $\vec{S}=\sum_{i \in \text { nucleus }} \vec{s}_{i}$, while the nuclear orbital angle moment is $\vec{I}=\sum_{i \in \text { nucleus }} \vec{I}_{i}$. This coupling results from the fact that interactions between the moments for a single particle are weak compared to interactions with other particles.

[^18]- Where the interaction between the spin angular moment and the orbital angular moment for a given particle is strong, the composition of the vectors is given by: $\overrightarrow{j_{i}}=\vec{s}_{i}+\vec{I}_{i}$ for each particle, and as the resulting total angular moment for the nucleus, $\vec{I}=\sum_{i \in \text { nucleus }} \overrightarrow{j_{i}}$.


### 1.13 Radioactivity

(Chelet 2006; Evans 1955; Guillien 1963; Halliday 1957; Munoz-Paez 2014; Pflaum 1992; Semat 1955)

It was the French physicist Claude Felix Abel Niepce ${ }^{24}$ (dubbed "de Saint Victor"), the germane cousin of famous photographer Joseph Nicéphore Niepce, who first demonstrated in the summer of 1857 and in the following years, the remote printing of photographic plates following their exposure by means of cardboard coated with a deposit of uranium salts. This print remained intact for a long time with the plate protected against light, but Niepce felt that it was necessary first to isolate the cardboard coated with uranium salt. He thought that a new unknown activity of light was involved that supposedly activated uranium, making it give up its radiation that was subsequently invisible, even in darkness. The chemist Michel-Eugène Chevreul, Dyes Manager at the Manufacture des Gobelins, who had had numerous exchanges with Niepce, understood the value of this discovery, and even used the term "activity" to describe the phenomenon.

[^19]However, Niepce remained a pioneer, and clearly a very important one, with regard to the discovery of radioactivity, although he did not understand the atomic nature of this phenomenon, since he continued to think that the action of light was necessary to provoke the invisible radiation. It is such tenuous details that separate the observer from the discoverer.

The discovery of radioactivity at the end of the nineteenth century gave an unprecedented boost to science in the fields of nuclear physics and particle physics. The secrets of the atom would be revealed within 50 years, and a mere 10 years after the discovery of the neutron, a reactor working on the principle of nuclear fission would already become a reality. Radioactivity was one field in which the French Physics establishment could feel particularly proud of itself. The end of the nineteenth century held out enormous hope, when in December 1895, the German physicist Wilhelm Conrad Roentgen (1845-1923) discovered $X$-rays (the $X$ in the name, although initially temporary, referred to the unknown nature of the rays, but because of its public success, the name was retained!) (Lowys 1925, p. 9), and in 1897, he produced the celebrated radiograph of his wife's right hand, which travelled around the world (Fig. 1.17).

The Nobel Prize for physics he was awarded in 1901 (the first such prize) for his discovery heralded the era of physicists investigating the structure of matter. The medical applications of this non-invasive method of investigation were immediately evident in traumatology. During the First World War, Marie Curie and her daughter Irène set up ambulances equipped with radiography devices enabling surgeons to diagnose problems and conduct operations extremely close to the battlefield (Loriot 1991, p. 157). The discovery of $X$-rays by Roentgen in late 1895, which was brought before the Académie des Sciences in a presentation by Henri Poincaré (1854-1912), led Henri Becquerel (1852-1908) to ponder on the


Claude Felix Abel Niepce (Public domain)


Fig. 1.17 The experimental equipment used by Roentgen to create an X-ray of his wife's hand in 1895-A Crookes tube is suspended above the hand, which is resting on a photographic plate
origin of the phosphorescence created in the vacuum tube under the effect of X-rays. Becquerel came from a family of celebrated researchers: his father, Edmond (1820-1891), had already studied the luminescence emitted by uranium compounds and the photovoltaic effect, and his grandfather, Antoine (1788-1878), had studied electrochemistry, climatology and physiology and had been a member of the "Académie des Sciences" (Photo 1.15).

Henri Becquerel investigated whether certain phosphorescent crystals might not be emitting $X$-rays. To this end, he placed phosphorescent salts exposed to natural light on a photographic plate. While handling a uranium salt, he discovered in February 1896 that a mark had been left on the plate without the salt being exposed to sunlight. ${ }^{25}$ He presented his results to the "Académie des Sciences" on February 241896 (Nahmias 1953, p. 12), and on reading his findings, it is clear that he still believed that sunlight had an effect on radiation.

However, in the text of his communication of March 2, 1896, it is very clear that he excluded the action of light in his procedure. His use of a gold foil electroscope enabled him to quantify the radioactivity because of its ability to discharge bodies

[^20]

Photo 1.15 Edmond Becquerel's dissertation on the analysis of light emitted by phosphorescent uranium compounds, Volume XL of the "Mémoires de l'Académie des Sciences", Firmin Didot, Paris, 1872, 40 pages. This text foretells the future discoveries of Henri Becquerel, although Edmond was unaware of anything but visible radiation! Edmond Becquerel also discovered the photovoltaic effect in 1839 but could not explain the cause (The Marguet collection)
initially carrying electrical charge. He determined that it was in fact uranium that was the emitter within the salt. He then set out the 5 laws of radioactivity. His sole mistake was to imagine that "uranic" rays could be reflected like light (which is not completely false if we take into account diffusion). Henri Becquerel established the key properties of radioactivity, namely: independence of the chemical form of the emitting uranium (solid, liquid, salts, etc.), independence of pressure, temperature, etc. (Photo 1.16).

Photo 1.16 Henri
Becquerel (1852-1908)
Discoverer of natural radioactivity, Nobel Prize for physics in 1903 together with Pierre and Marie Curie (Nobel Prize photo, Public domain)


Radioactivity was considered a new property of matter independent of any outside conditions. He was awarded the Nobel Prize in 1903 together with Pierre and Marie Curie. This discovery opened up an extremely fertile period for French science: in 1898, Pierre (1859-1906) and Marie Curie (1867-1934) isolated polonium from pitchblende, followed by radium ${ }^{26,27,28}$ (Dupuy 1962). Pierre and his brother Jacques were already known after their discovery of the piezoelectric effect in 1880 (Barbo 2005, p. 11). Pierre was a specialist in metrology and developed a "balance" enabling extremely precise measurement of radioactivity based on the propensity of the latter to discharge electrified bodies.

Marie Curie experimentally determined the atomic weight of ${ }_{88}^{226} R a$ as being $225 \pm 1$ (it is in fact 226), ${ }^{29}$ which was an astonishing feat for the time, given the very small amount of pure substance at her disposal. Very quickly, the Curies provided industry with a technique for the separation of radium without taking out a patent, and many foreign laboratories (including Rutherford's laboratory) were kindly supplied with radium by the Curies (Photo 1.17).

She also measured its half-life: 1600 years $\pm 7$ years. The excellent French theater play "Les Palmes de Mr Schutz" gives a clear impression of the miserable

[^21]

Photo 1.17 An uncommon photograph (although its rather bad quality) of Marie Curie in her laboratory at the "Faculté des Sciences", Paris, circa 1910 (from "La science et la Vie, January 1914, Public domain)
working conditions of Pierre and Marie Curie, who labored tirelessly to understand the source of radioactivity from pitchblende. According to the play, the housemaid has the idea that the infinitely small residues from the separation efforts might contain the radioactivity found in the entire mineral. Unfortunately, Pierre Curie died in a senseless accident, being crushed under the wheels a horse-drawn cart in a Paris street in 1906, leaving Marie to continue the research on radioactivity. Thanks the increasing availability of radium (Marie Curie generously supplied radium to a number of laboratories for study purposes), physicists throughout the world were able to study radioactivity. Ernest Rutherford (1871-1937) devoted all his energy to this end, identifying several types of radiation, which he simply termed $\alpha, \beta$ and $\gamma$ radiations (Photo 1.18).

Rutherford and his assistant Frederick Soddy (1877-1956) observed changes in the chemical properties of the emitter of $\alpha$ and $\beta$ rays, namely transmutation. Not all natural isotopes are radioactive. Rutherford is credited with being the first to speculate on what today appears obvious: the heaviest isotopes are the most unstable. It was Rutherford who identified the $\alpha$ particle as a nucleus of helium 4. Between 1908 and 1910 while in Manchester, Rutherford and his pupil Hans Geiger measured to within $10 \%$ the values currently accepted today for the radioactive half-lives of ${ }^{226} R a,{ }^{232} T h,{ }^{238} U$ and ${ }^{235} U$ (Birks 1961). He was the first to use measurement of the quantity of helium trapped in radioactive minerals such as pitchblende to estimate, in 1905, the age of formation of these minerals. These measurements, which showed certain minerals to be over 700 million years old, revolutionized ideas about the age of the Earth, creating a (false) controversy with Lord Kelvin, whose calculations for pure radiation from a sphere in a vacuum suggested that the Earth had existed for around 100 million years and would


Photo 1.18 Pierre and Marie Curie as viewed by the theatre (courtesy of l'Avant-Scène Théâtre)
continue to exist for a similar period. ${ }^{30}$ This method of determining the chronological age of minerals was further developed in 1907 by Bertram B. Boltwood (1870-1927), who noted that lead results from the disintegration of uranium, and

[^22]that as a result, the ratio of lead to radium in rocks was increasing over time. The phenomenon is correlated with age. In 1913, Rutherford observed that solar energy could not be accounted for by only the radioactivity of heavy nuclei. He calculated that if the sun were a sphere of pure uranium, it would in fact emit no more than a quarter of the energy actually emitted by radiation. He explained this by postulating that the sun must fully utilize all of the energy contained within the light atoms, thus predicting fusion. By the deflection of $\alpha$ particles, Rutherford also determined that the electrical charge on an atom is concentrated within the nucleus, whose mass number appears greater than the charge number. In 1920, Rutherford thus postulated the extra distance of an electrically neutral particle: the neutron. In 1930, Walter Bothe (1891-1957) and H. Becker, ${ }^{31}$ then Frédéric Joliot (1900-1958) and his wife Irène Curie (1897-1956), noted that the bombardment with $\alpha$ rays of light nuclei such as beryllium, produced highly penetrating radiation. ${ }^{32}$ Until then, highly energetic $\gamma$ rays had been considered-wrongly as it turns out. It was finally James Chadwick who in 1932 correctly interpreted the experiment ${ }^{33}$ and won the Nobel Prize in 1935:
$$
\alpha+{ }_{4}^{9} \mathrm{Be} \quad \rightarrow \quad{ }_{6}^{12} \mathrm{C}+{ }_{0}^{1} n+5 \quad \mathrm{MeV}\left(\alpha \text { : helium nucleus }{ }_{2}^{4} H e^{2+}\right)
$$

Highly penetrative radiation thus comprised neutrons. In 1934, Frédéric and Irène Joliot-Curie discovered artificial radiation ${ }^{34}$ on bombarding an aluminum sheet with $\alpha$ particles:

$$
{ }_{2}^{4} \mathrm{He}+{ }_{13}^{27} \mathrm{Al} \rightarrow{ }_{15}^{30} \mathrm{P}+{ }_{0}^{1} n
$$

The phosphorus atom ${ }_{15}^{30} P$ does not exist naturally and it is thus an artificial nucleus that disintegrates by radioactivity:

$$
{ }_{15}^{30} P \rightarrow{ }_{14}^{30} S i+{ }_{1}^{0} e^{+} T=1.7 \mathrm{~min}
$$

They received the Nobel Prize for physics in 1935 for the discovery of artificial radioactivity. Since then, some 1000 artificial isotopes have been created! Radioactivity is a spontaneous phenomenon of a statistical nature for which binomial distribution may be demonstrated (Uhrig 1970, p. 27) since it is possible to calculate the probability that $M$ atoms produced by $N$ initial atoms disintegrate in time $t$ according to the following formula:

[^23]$$
p(M)=\frac{N!}{(N-M)!M!} p^{M}(1-p)^{N-M}
$$
where $p$ is the probability that the first of $M$ atoms disintegrates at time $t .1-p$ is thus the probability that an atom will not have disintegrated at time $t$. In this expression, we recognize the binomial coefficient $C_{N}^{M}=\binom{N}{M} \equiv \frac{N!}{(N-M)!M!}$ which is reasonably understandable as we are seeking to determine the number of possibilities of selecting the first atom to disintegrate among the $N$ possible atoms, followed by the second among the $N-1$ possible atoms, and so on, until all of the $M$ atoms available for disintegration have been used up. Radioactivity is completely independent of external conditions (e.g. pressure, time) and is subject to Becquerel's law:
\[

$$
\begin{equation*}
\text { Becquerel's law for radioactive decay: } \frac{d N}{d t}=-\lambda N \tag{1.4}
\end{equation*}
$$

\]

where: $N$ is the number of nuclei of the radioactive isotope (may also be by volume units); $\lambda$ is the radioactive decay constant of the radioisotope (unit: $\mathrm{s}^{-1}$ ); $t$ is time [ s$]$.

If there are $N_{0}$ atoms present at time $\mathrm{t}_{0}$, integration of the above expression gives:

$$
N=N_{0} e^{-\lambda\left(t-t_{0}\right)}
$$

Taking $t_{0}=0$ as the time origin, we have: $N=N_{0} e^{-\lambda t}$.
By the definition of $p: p \equiv 1-\frac{N(t)}{N_{0}}=1-e^{-\lambda t}$ the mean number of disintegrations occurring over time $t$ is given by (Uhrig 1970, p. 28):

$$
\begin{aligned}
\mu & =\sum_{M=0}^{N_{0}} M p(M)=\sum_{M=0}^{N_{0}} M \frac{N_{0}!}{\left(N_{0}-M\right)!M!} p^{M}(1-p)^{N_{0}-M} \\
& =N_{0} p(p+(1-p))^{N_{0}-1}=N_{0} p
\end{aligned}
$$

In the event of an extremely high initial number of atoms $N_{0}$ and where the sample $M$ is very small in relation to $N_{0}$, the formula for $p(M)$ may be simplified where $p=1-e^{-\lambda t} \approx \lambda t$, using Stirling's formula to approach the factorial:

$$
\begin{align*}
& \text { Stirling's formula: } n!\approx \sqrt{2 \pi n} e^{-n} n^{n}  \tag{1.5}\\
& \text { Under these hypotheses: } \quad p(M)=\frac{\mu^{M}}{M!} e^{-\mu}
\end{align*}
$$

which is in fact a Poisson distribution. Turning now to $M$ of an extremely high value, and using:

$$
\operatorname{In}\left(\frac{\mu}{M}\right)=\operatorname{In}\left(1+\frac{\mu-M}{M}\right) \approx \frac{\mu-M}{M}-\frac{(\mu-M)^{2}}{2 M^{2}}
$$

Gaussian distribution is obtained:

$$
p(M)=\frac{1}{\sqrt{2 \pi \mu}} e^{-\frac{(\mu-M)^{2}}{2 \mu}}
$$

The term half-life or half-life period denotes the time required for half of the radioactive atoms initially present to decay.

$$
N(T)=\frac{N_{0}}{2}
$$

The half-life of a particular isotope is given by:

$$
\begin{equation*}
\text { Half-life of radioactive decay: } T \equiv \frac{\operatorname{In} 2}{\lambda} \approx \frac{0.693}{\lambda} \tag{1.6}
\end{equation*}
$$

After 10 half-lives, the remaining amount of radioactivity is generally considered negligible as:

$$
N(10 T)=\frac{N_{0}}{2^{10}}=\frac{N_{0}}{1024}
$$

The "stability" of a given nucleus is in fact dependent upon the precision of our measuring instruments. If the half-life is too long, decay becomes so slight that it may be masked by background noise and the nucleus is seen as stable. Similarly, below $10^{-20} \mathrm{~s}$, the nuclei are too unstable to be able to be studied today. These nuclei are investigated chiefly thanks to their daughter nuclei. The term mean lifetime $\theta$ refers to the time after which the number of radioactive atoms is reduced by Euler's number, $e$.

$$
\begin{gathered}
N(\theta)=\frac{N_{0}}{e} \\
\theta=\frac{\int_{0}^{\infty} t N(t) d t}{\int_{0}^{\infty} N(t) d t}=\frac{\int_{0}^{\infty} t N_{0} e^{-\lambda t} d t}{\int_{0}^{\infty} N_{0} e^{-\lambda t} d t}=\frac{1}{\lambda}
\end{gathered}
$$

The activity $A(t)$ of a radioactive nucleus is defined as the number of decays or disintegrations per second, in other words, radioactivity is given by:

$$
\begin{equation*}
\text { Activity of a radioactive isotope: } A(t) \equiv \lambda N(t) \tag{1.7}
\end{equation*}
$$

Since 1975, the official unit of radioactivity has been the Becquerel $(\mathrm{Bq}) \equiv 1$ disintegration. $\mathrm{s}^{-1}$. Where the concentration of an isotope is given in volume units, the volume activity is expressed in $\mathrm{Bq} / \mathrm{cm}^{3}$. For convenience, for the levels of radioactivity normally found, we use a more suitable unit far higher than the Bq : the Curie. $1 \mathrm{Ci}=3.7010^{10} \mathrm{~Bq}$. This is the activity of 1 gram of radium 226 (beware: radium not curium!). For example, one metric ton of natural uranium contains 1 Ci of ${ }^{234} U, 1 \mathrm{Ci}$ of ${ }^{238} U$ and 0.5 Ci of ${ }^{235} U$. The half-life of radium 226 is $1600.04 \pm 7.0014$ years. Methods of measuring of radioactive half-lives have become so accurate that they are
used today in defining reference units such as seconds and even meters. The standard meter, the universal reference for the measuring unit, which is piously kept at the Museum of Weights and Measures in Sèvres (France), just outside Paris, was initially made out of platinum-iridium alloy (accurate to within a 100th of a micron!). However, even this rare alloy is sensitive to both thermal expansion and pressure. From 1962 to 1983, the new definition of the meter was in fact based upon a form of decay readily accessible to researchers, namely that of krypton 86 .

$$
1 \text { meter } \equiv 1650763.73 \times \lambda_{2 \mathrm{P} 10->5 \mathrm{D} 5} \text { of }{ }_{36}^{86} \mathrm{Kr}
$$

Since 1983, progress in measuring the speed of light in a vacuum ( $299,792,458 \mathrm{~m} / \mathrm{s}$ ) means that the value of the meter may be defined in terms of the latter, with 1 meter being the distance travelled by light in a vacuum in 1/299,792,458 seconds.

### 1.13.1 Alpha Decay

(Lilley 2001, p. 84)
Alpha decay was the first type of radioactivity to be discovered since the alpha particle is emitted by most radioactive heavy isotopes (uranium, radium, radon, etc.). It was Ernest Rutherford who identified the $\alpha$ particle as a helium nucleus thanks to the skill of his glassblower, who created a glass tube with thin double walls. A vacuum was created between the two walls and $\alpha$ particles fired from a source located inside the first tube caused helium gas to appear in the space between the walls which was initially "filled" with vacuum. The first effective sources of $\alpha$ particles were created from radium purified by the technique of Pierre and Marie Curie (Photo 1.19). Alpha radiation is produced by the ejection of a helium nucleus:

$$
\begin{equation*}
\text { Alpha decay: }{ }_{Z}^{A} X \rightarrow{ }_{Z-2}^{A-4} Y+{ }_{2}^{4} H e^{+2 e} \tag{1.8}
\end{equation*}
$$

The emission of an $\alpha$ particle can be depicted schematically in an energy diagram, as in Fig. 1.18. It should be noted that emission does not necessarily result in the production of a nucleus in its ground state and that $\gamma$ photons are frequently emitted. It was Salomon Rosenblum ${ }^{35}$ (1896-1960) who in 1929 first demonstrated

[^24]the fine structure of $\alpha$ radiation from Thorium $C$ (the name used at the time for bismuth 212), consisting of 4 rays, ${ }^{36}$ using magnetic methods (Rosenblum 1932; Rosenblum 1969, p. 7) (Figs. 1.19, 1.20, 1.21 and 1.22).

Until then, it had been thought that the $\alpha$ emission by a radio-isotope was monokinetic. Rosenblum thus discovered that the associated $\gamma$ radiation obeyed the same laws as the rearrangement of electron shells, in other words that the energy of the photons emitted corresponded to the difference in energy in the emissions of $\alpha$ particles, demonstrating that quantum theory also applies to the energy levels of the nucleus. For example, the decay of ${ }_{90}^{228} T h$ is as follows:

[^25]

Experiments on neutrons in some cave in Bellevue laboratories -Public domain
${ }^{36}$ Salomon Rosenblum: Structure fine du spectre magnétique des rayons alpha du thorium [Fine structure of the magnetic spectrum of alpha rays from thorium], Comptes-rendus de l'Académie des Sciences, No 188, pp. 1401-1403 (1929)


LES SELS RADIOACTIFS SONT TRAITÉS DANS DES RÉCIPIFNTS DE PLES EN PLES PETITS Les solutions ale bromure de radium radifire sont doucement rivapories dans des marmites en fer tmailld dont le fond se recouvre de cristaux. On sépare les dispdts successifs.


A L'Usine de mogent, C'est tne chimiste qui fait les nekniers fractionntments Les cristallisations /ractionntes qui permettent de sfparer progressivement le bromure de vadium du bromure do baryum s'effectuent dans des capsules chauffies au gax.

Photo 1.19 Chemical preparation of radium at the beginning of the twentieth century in the factory of Nogent-sur-Marne, France. Radium is dissolved with some bromide of barium, the barium having chemical properties similar to the radium, then the bromide of radium is separated from the bromide of barium by the method of the split crystallizations (adapted from "La Science


Fig. 1.18 The piezo-electric balance invented by Pierre Curie. The idea is to counter-balance the electricity produced by a standard weight stretching a piece of quartz (circa 1904)


Fig. 1.19 The capacitor discharge technique: radioactive material is put on the trays made of brass of the capacitor, trays are isolated with amber from the rest of the apparatus. The supporting tray is previously charged from a battery and the operator measures the time of discharge (circa 1910, Public domain)

Photo 1.19 (continued) et la Vie" of January, 1914, Public domain). One can expect radioprotection problems by handling concentrated solutions of radium with no gloves !, The factory of Nogent was built by Emile Armet de l' Isle (1853-1928) and it was the first one to the world as soon as 1904 to produce radium salts by using the process of the Curie with whom he works closely. Armet de l'Isle also initiated the prestigious scientific journal "The Radium"

Fig. 1.20 The gold foil electroscope: the idea is to measure the speed of the discharge of a previously charged gold foil (by looking at the movement of the foil in front of a reticular). The operator must have a pair of sharp eyes and a precise chronometer! (circa 1910, Public domain)

Fig. 1.21 Radioactive decay of an isotope of initial concentration $N_{0}$


Fig. 1.22 Energy diagram of $\alpha$ decay



Fig. 1.23 Decay scheme of ${ }_{88}^{226} R a$


Fig. 1.24 Wave function of an $\alpha$ particle in the Coulombic field of a nucleus

$$
\left\{\begin{array}{lll}
{ }^{228} \mathrm{Th} & \rightarrow & { }_{88}^{224} \mathrm{Ra}+{ }_{2}^{4} \mathrm{He}^{+2 e}+E_{\alpha} \\
{ }_{20}^{224} R a & \rightarrow & { }_{82}^{220} R n+{ }_{2}^{4} \mathrm{He}^{+2 e}+E_{\alpha} \\
{ }_{88} R \text { Metal }
\end{array}\right)
$$

The term $E_{\alpha}$ denotes all decay energy, whether in the form of recoil kinetic energy of the isotope formed, kinetic energy from the $\alpha$ particle itself, or energy from the photon(s) emitted. Figure 1.23 gives a decay diagram showing several modes of disintegration of ${ }_{88}^{226} R a$.

A considerable percentage of disintegration results in an excited level of ${ }_{86}^{222} R n$ and in the emission of a de-excitation photon. Where there are several photons corresponding to several different modes, we obtain an emission spectrum quantified by the excitation states of the daughter nucleus. Alpha radiation involves "heavy nuclei" ( $Z \geq 82$, actinides and rare earth elements) with the exception of one or two fission products such as ${ }^{144} N d$, which emits a particle at 1.9 MeV with a half-life of $510^{15}$ years. According to the laws of classical mechanics, no $\alpha$ particles of less than 20 MeV should be able to cross the Coulomb barrier (Fig. 1.24).

However, the $\alpha$ energy emitted by $\alpha$ radioactivity is of the order of $4-5 \mathrm{MeV}$. The explanation for this apparent contradiction is that the wave function $\Psi$ of $\alpha$


Fig. 1.25 Trajectory of $\alpha$ particles in dry air
particles of 4 MeV has non-zero values outside the potential well, enabling the expulsion of the $\alpha$ particle. This occurs through the tunnel effect (Fig. 1.25).

Max Born (1882-1970), Nobel prizewinner in 1954, showed that the probability of the presence of a particle was proportional to the square of the wave function. If the wave function of the particle is not zero outside the potential well of the heavy nucleus, it can overcome the barrier: this is known as the tunnel effect or tunneling. The emission spectrum of $\alpha$ particles is inherently discontinuous (ray spectrum). Alpha particles take with them an energy that maybe calculated if the initial and final energy levels of the nucleus are known. If the resulting level is above the ground state, de-excitation occurs via $\gamma$ radiation. In some cases, the spectrum may be reduced to a single ray, as with uranium 235 , which emits only $\alpha$ particles at 4.5 MeV. Alpha particles are charged and heavy ( $3729 \mathrm{MeV} / c^{2} \approx 4$ uma), and are therefore quickly stopped and absorbed in situ, or they may be stopped by a thin aluminum sheet. Even air is sufficient to stop $\alpha$ radiation within a few tens of centimeters. In uranium oxide, emission of an $\alpha$ particle results in the displacement of around 150 atoms, although the recoil of the emitting nucleus (of the kinetic energy of 100 keV ) results in displacement of around 1500 atoms, due to its far greater mass.

It is possible to determine from the energy balance whether or not disintegration can occur.
which is possible where $M_{X}-M_{Y} \geq M_{\alpha}$. In terms of binding energy, this results in:

$$
E_{\text {Binding } X}-E_{\text {Binding } Y} \leq E_{\text {Binding } \alpha}=28.33 \mathrm{MeV}
$$

With long emission periods, the energy of alpha particles is low, and vice versa. This is the Geiger-Nuttal law.

### 1.13.2 $\beta^{-}$Decay

(Konopinski 1966; Lilley 2001, p. 74)
$\beta^{-}$decay is an isobaric transformation in which the number of nucleons is conserved. A nuclear neutron is transformed into a proton through the emission of an electron and an antineutrino.

$$
{ }_{0}^{1} n \rightarrow{ }_{1}^{1} p+{ }_{-1}^{0} e^{-}+\bar{\nu}
$$

In its free state, a neutron is itself $\beta^{-}$radioactive, with a half-life of 12.8 minutes and 783 keV of liberated energy. Inside the nucleus, however, the neutron "loses" this property and the radioactivity of the isotope is no longer dependent upon that of the neutron, but it has its own half-life.

$$
\begin{equation*}
\beta^{-} \text {decay: }{ }_{Z}^{A} X \rightarrow{ }_{Z+1}^{A} Y+{ }_{-1}^{0} e^{-}+E_{\beta^{-}} \tag{1.9}
\end{equation*}
$$

A point of interest to reactor physicists is the existence of a very rare form of decay known as double beta decay, which poses the twin problem of the emission and mass of neutrinos; it is also of historical value since it enabled the discovery of non-conservation of parity (Klapdor-Kleingrothaus 2001):

$$
{ }_{Z}^{A} X \rightarrow{ }_{Z+2}^{A} Y+{ }_{-1}^{0} e^{-}+{ }_{-1}^{0} e^{-}
$$

An important example of $\beta^{-}$decay in reactor physics is that of ${ }_{94}^{241} P u$, a fissile isotope, which produces the isotope ${ }_{95}^{241} \mathrm{Am}$, an important neutron absorber. This phenomenon, known as americium build-up, poisons plutonium, requiring the loading of corresponding fissile quantities into the reactor due to the inevitable ageing that occurs between the reprocessing phase and the manufacturing phase of mixed oxide fuel comprising $\mathrm{UO}_{2}$ and $\mathrm{PuO}_{2}$ (MOX).

$$
{ }_{94}^{241} \mathrm{Pu} \rightarrow{ }_{95}^{241} \mathrm{Am}+{ }_{-1}^{0} e^{-}+E_{\beta^{-}} \quad \text { Half-life } T=14.4 \text { years. (JEF } 2 \text { ) }
$$

It should be noted that the decay of ${ }_{19}^{40} K$, which is present in the human body (its massic abundance in natural potassium, is ${ }_{19}^{40} K / K_{\text {total }}=0.01 \%$ ):

$$
{ }_{19}^{40} K \rightarrow{ }_{20}^{40} \mathrm{Ca}+{ }_{-1}^{0} e^{-} \quad T=1.210^{9} \text { years. }
$$

The decay of tritium, a hydrogen isotope containing 3 nucleons, which poses radioprotection problems in $P W R s$ due to its extreme propensity for migration, is:

$$
\underset{\text { Tritium }}{{ }_{1}^{3} \mathrm{H}} \rightarrow \underset{\text { Helium } 3 \text { highly absorbant }}{{ }_{2}^{3} \mathrm{He}}+{ }_{-1}^{0} e^{-}
$$

Beta decay is the most common form of radioactivity; in particular, the majority of fission products emit $\beta^{-}$radiation. It is thus the primary cause of residual power in nuclear reactors following shutdown (or scram). If we evaluate the total decay energy $Q$ of the decay ${ }_{Z}^{A} X \rightarrow{ }_{Z+1}^{A} Y+{ }_{-1}^{0} e^{-}+E_{\beta^{-}}$by mass defect $\left(M_{X}-M_{Y}-m_{e^{-}}\right) c^{2}, Q$ is consistently equal to the maximum energy of the emitted electrons, while experimentally, a spectrum continuous in energy up to $E_{\text {max }}$ is emitted.

The question of what happens to the difference $E_{\max }-E$ puzzled physicists for a long time, to the extent that some even doubted the principle of conservation of energy. It was Enrico Fermi who first proposed a theory of $\beta$ decay based on the existence of the neutrino ${ }^{37}$ ("little neutron" in Italian), which is known today as the electron antineutrino $\bar{\nu}$ (Fig. 1.26).

This particle, which is neutral and apparently of zero mass (despite numerous experiments, it has still proved impossible to determine whether the mass is in fact pure zero), carries away on average around $2 / 3$ of the energy of the process. Because of its inherent characteristics, this particle is extremely difficult to detect (no-mass particles poorly interact), since out of every $10^{10}$ neutrinos or more reaching and passing through the planet Earth from space, only one will be captured (by the process: $\bar{\nu}+{ }_{1}^{1} p \rightarrow{ }_{0}^{1} n+{ }_{1}^{0} e^{+}$). For a neutrino not subject to electromagnetic force and of infinitesimal or even zero mass, matter is practically transparent. Enrico Fermi's work on $\beta$ decay won him the Nobel Prize in 1938. The total energy of $\beta^{-}$decay, $Q_{\beta^{-}}$, is given by the following mass equation:


Mass $M(Y)$ contains only $Z$ electrons since it is the disintegration of the neutron that produces the new electron emitted: ${ }_{0}^{1} n \rightarrow{ }_{1}^{1} p+{ }_{-1}^{0} e^{-}+\bar{\nu}$, and atomic mass $Y$ is by definition the mass of the neutral atom containing $Z+1$ electrons, so that:

[^26]Fig. 1.26 Example of a $\beta^{-}$ decay scheme: the $\beta^{-}$decay of ${ }_{13}^{28} \mathrm{Al}$ produces ${ }_{14}^{28} \mathrm{Si}$

$$
\underset{\mathrm{Z} \text { electrons }}{M(Y) c^{2}}=\underbrace{M(Y) c^{2}}_{\text {Atomic Mass }(Y, A) \mathrm{c}^{2}} \operatorname{Mith}_{\mathrm{Z}+1 \text { electrons }}^{\text {wic }}-m_{e^{-}} c^{2}
$$

Hence:

$$
Q_{\beta^{-}}=\left[M_{\text {atomic }}(Z, A)-M_{\text {atomic }}(Z+1, A)\right] c^{2}
$$

This energy cannot be completely recovered since the kinetic energy of the neutrinos is lost (as neutrinos interact very little with matter). An interesting case of $\beta^{-}$decay is that of ${ }_{6}^{14} C$ (carbon-14) and its applications in carbon dating (Annual review of nuclear science Vol. 2 1953, p. 63). Isotope ${ }_{6}^{14} C$ is formed following the capture by ${ }_{7}^{14} N$ of secondary neutrons due to bombardment by cosmic rays (Annual review of nuclear science Vol. 2 1953, p. 335), (Valentin 1982a, b, p. 78; Progress in nuclear physics Vol 8 1960a, b, p. 1):

$$
\begin{equation*}
\text { Production of }{ }_{6}^{14} C:{ }_{0}^{1} n+{ }_{7}^{14} N \rightarrow{ }_{6}^{14} C+{ }_{1}^{1} H+0.62 \mathrm{MeV} \tag{1.10}
\end{equation*}
$$

Isotope ${ }_{6}^{14} C$ is thus present in natural carbon, but consists of $\beta^{-}$radiation with a half-life of $5730 \pm 40$ years (JEF2).

$$
{ }_{6}^{14} C \rightarrow{ }_{7}^{14} N+{ }_{-1}^{0} e^{-}
$$

If bombardment is constant, the quantity of ${ }_{6}^{14} \mathrm{C}$ in carbon dioxide is also constant. Living creatures, which continually exchange with the $\mathrm{CO}_{2}$ atmosphere through breathing, also have a constant level that diminishes after their death (cessation of breathing), and it is this phenomenon that forms the basis of ${ }_{6}^{14} C$ dating. It should be noted that this method may be used to investigate only a very short time period (between today and some 100,000 years in the past), which is far less than the age of our planet. It was Willard F. Libby (1908-1980), the Nobel Prize winner for chemistry in 1960, who developed carbon dating at the end of the 1940s with the assumption that the ${ }_{6}^{14} C /{ }_{6}^{12} C$ ratio remains constant in the atmosphere over time. It should also be noted that only living organisms actually participating in the carbon cycle may be dated (wood, bone, plant and animal tissue, etc.). Minerals and metals cannot in any event be dated using this technique (regarding specific problems with dating, see (Radioactive dating 1967)). In practice, in comparison with other dating methods (geological strata, dendrochronology consisting of counting the number of rings in trees, extraction of ice samples from deep below the Arctic surface), it has been shown that concentrations of ${ }_{6}^{14} C$ have
not always been constant over the centuries. This is due primarily to the fact that the Earth's magnetic field has varied throughout the course of history (the stronger the magnetic field, the less the ability of charged particles to reach the high atmosphere and produce ${ }_{6}^{14} C$ ). Important progress has been made in ${ }_{6}^{14} C$ dating using the Tandetron, a mass spectrometer coupled with a tandem accelerator. In particular, AMS (Accelerator Mass Spectrometry) allows direct reading of the ratio of ${ }_{6}^{14} \mathrm{C} /{ }_{6}^{12} \mathrm{C}$ without having to wait a long time for the threshold for counting of ${ }_{6}^{14} \mathrm{C}$ disintegrations to be reached when seeking to measure very old materials. The sample size necessary for measurement by Tandetron is around 1 mg . It has thus been possible to date the prehistoric paintings in the Cosquer Cave near Cassis in the south of France to around 20,000 years, without harming the originals in any. We thus have extremely precise historical data on the abundance of ${ }_{6}^{14} \mathrm{C}$ in the atmosphere, reliable to a time 9000 years ago, thanks to comparative studies using dendrochronology. For earlier times, lake sediments presenting seasonal alternation enable comparison, although more widely dispersed, until 25,000 years ago.

### 1.13.3 $\quad \beta^{+}$Radioactivity

(Konopinski 1966)
On transformation into a neutron, a nuclear proton emits a positron, $e^{+}$(positive electron, (Valentin 1982a, b, p. 78)), and a neutrino (Fig. 1.27):

$$
{ }_{1}^{1} p \rightarrow{ }_{0}^{1} n+{ }_{1}^{0} e^{+}+v
$$

Applied to the nucleus, this expression may be written as follows:

$$
\begin{equation*}
\beta^{+} \text {decay: }{ }_{Z}^{A} X \rightarrow{ }_{z-1}^{A} Y+{ }_{1}^{0} e^{+}+E_{\beta^{+}} \tag{1.11}
\end{equation*}
$$

The total decay energy, $Q_{\beta^{+}}$, is given by the mass equation:

Fig. 1.27 Example of a $\beta^{+}$ decay scheme


$$
\underset{\text { with Z electrons }}{M(X) c^{2}}=\underset{\text { with Z electrons }}{M(Y) c^{2}}+m_{e^{+}} c^{2}+\underbrace{E_{\text {recoil }}^{Y}+\underbrace{E_{\text {kin }}^{e^{+}}+E_{k i n}^{\nu}}_{E_{\max }}+E_{\gamma}}_{Q_{\beta^{+}}}
$$

since a positron occurs through decay of a proton: ${ }_{1}^{1} p \rightarrow{ }_{0}^{1} n+{ }_{1}^{0} e^{+}+\nu$ as follows:

$$
\underset{\text { with Z electrons }}{M(Y) c^{2}}=\underbrace{\text { with } Z-1 \text { electrons }}_{M_{\text {atomic }}(Z-1, A)} \quad M(Y) c^{2}+m_{e^{-}} c^{2}
$$

and the mass of the electron is identical to that of the positron, we see that:

$$
Q_{\beta^{+}}=\left[M_{\text {atomic }}(Z, A)-M_{\text {atomic }}(Z-1, A)-2 m_{e}\right] c^{2}
$$

### 1.13.4 Electron Capture

A peripheral electron bound to an atom (often an electron in the $K$ shell) will combine with a proton located in the nucleus to give a neutron:

$$
\left({ }_{-1}^{0} e^{-}\right)_{A_{Z} X}+{ }_{Z}^{A} X \rightarrow{ }_{Z-1}^{A} Y+\text { Xray }
$$

This phenomenon is explained by the capture of an electron by a nuclear proton (Fig. 1.28):

$$
{ }_{-1}^{0} e^{-}+{ }_{1}^{1} p \rightarrow{ }_{0}^{1} n
$$

The resulting electron rearrangement leads to X-ray emission characteristic of element $Y$. The mass number is conserved. Electron capture produces the same isotope as $\beta^{+}$decay, albeit through an entirely different process.

$$
\left({ }_{-1}^{0} e^{-}\right)_{7_{4}^{7} B} e+{ }_{4}^{7} B e \rightarrow{ }_{3}^{7} L i+E_{X}
$$

Fig. 1.28 Decay scheme of electron capture of ${ }_{4}^{7} \mathrm{Be}$


### 1.13.5 $\gamma$ Radioactivity

Photon emission, discovered in 1900 by Paul U. Villard, ${ }^{38}$ is the most common way in which an atomic nucleus loses its energy (compared with other types of radioactivity which are possible for metastable nuclei) (Fig. 1.29).

Although the probability of transition from the first excited nuclear state to the ground state is relatively small, this corresponds to a period sufficiently long to be measurable. The term nuclear photon is used to describe such photons emitted by a nucleus to distinguish them from photons emitted by rearrangement of an electron shell, which are referred to as $X$-rays or visible light. In this case, an excited isotope is said to be metastable, and the excited and fundamental isotopes are isomers. The $\gamma$ radiation of nuclear de-excitation is thus a form of electromagnetic radiation identical to visible radiation but occurring at a lower wavelength. The decay equation is as follows:

$$
\begin{equation*}
\gamma \text { decay: }{ }_{Z}^{A} X^{*} \rightarrow{ }_{Z}^{A} X+E_{\gamma} \tag{1.12}
\end{equation*}
$$

For example, the $\gamma$ decay of the isotope ${ }_{95}^{242 m} \mathrm{Am}$, an isomer of ${ }_{95}^{242} \mathrm{Am}$, is as follows:

[^27]
(Public domain)

Fig. $1.29 \gamma$ decay scheme

The index $m$ denotes metastable, in other words a specific excited state. For more excited states the indices $n, o$, etc. are used. It is not impossible for certain excited states to have longer half-lives than the ground state. Where there may be any doubt, the terms short life and long life are used to distinguish between two such isotopes, as for example with the isotopes ${ }_{93}^{236} N p_{\text {long }}$ and ${ }_{93}^{236} N p_{\text {short }}$. Care should be taken to avoid confusing this nuclear de-excitation due to photons with the emission of a photon due to quantum leap, which is not a form of radioactivity.

### 1.13.6 Internal Conversion

(Kaplan 1956, p. 298)
A nucleus in an excited state generally releases energy through the emission of a photon in the event of $\gamma$ radioactivity; however, this energy may also be transferred to a bound electron that is ejected and generally emits an X-ray photon due to rearrangement of the electron shell, with the transfer of kinetic energy $E_{0}-E_{L}$ where $E_{0}$ is the available excitation energy and $E_{L}$ is the binding energy of the electron thus ejected.

The term conversion electron is used for the ejected electron. Up to 8 different conversion rays can be seen (Fig. 1.30).

This phenomenon leads to electrons having highly specific energies, while $\beta^{-}$ emission produces a continuous spectrum. These discrete rays are superimposed in the continuous spectrum when $\beta^{-}$radioactivity leaves the isotope in an excited state enabling internal conversion (Lilley 2001, p. 71). As an example, consider metastable ${ }_{56}^{137 *} B a$ with a half-life of 2.55 minutes. The isotope resulting from the internal conversion is fundamental but ionized barium (Fig. 1.31):

$$
{ }_{56}^{137 *} B a \rightarrow{ }_{56}^{137} B a^{+}+{ }_{-1}^{0} e^{-}
$$

Internal conversion is only really important for low-energy transitions in heavy nuclei. If a nucleus has an excitation energy greater than 1.022 MeV that it is unable to release:

- by means of internal conversion, since it is forbidden by a quantum selection rule,
- or by emission of a photon through $\gamma$ decay.


Fig. 1.30 Decay scheme of ${ }_{56}^{137 *} B a$


Fig. 1.31 Internal conversion. (a) Energy transferred to an ejected electron. (b) Rearrangement of the electron shell and emission of an $X$ photon

An electron-positron pair may be formed (Filippi 1965, p. 224), which will carry away the residual energy as kinetic energy (Berthelot 1956, p. 117). Here, the term internal materialization is used to denote a phenomenon comparable with the creation of an electron-positron pair when a photon passes through an electromagnetic field.

### 1.13.7 ( $\boldsymbol{\beta}^{-}$,n) Decay or Neutron Decay

$\left(\beta^{-}, n\right)$ decay, which occurs with radioactive fission products with a particularly high excess of neutrons, combines simultaneous emission of an electron ( $\beta^{-}$) and a neutron. The neutrons thus produced are known as delayed neutrons, since they are not emitted instantaneously after fission but according to the radioactive half-life of ( $\beta^{-}, n$ ) decay specific to the fission product.

$$
\begin{equation*}
\left(\beta^{-}, n\right) \text { decay: }{ }_{Z}^{A} X \rightarrow{ }_{Z+1}^{A-1} Y+{ }_{-1}^{0} e^{-}+{ }_{0}^{1} n+E_{\beta^{-}} \tag{1.13}
\end{equation*}
$$

$\left(\beta^{-}, n\right)$ decay is also known as neutron decay, a relatively imprecise term that can cause confusion, particularly since the neutron is itself radioactive in the free state, a good reason to avoid the use of such term.

### 1.13.8 Spontaneous Fission

(Mayo 1998, p. 215)
This occurs with very heavy nuclei such as ${ }_{98}^{252} C f$ (californium). The heavy nucleus naturally splits into two lighter parts due to tunneling (passage over the fission barrier) while also emitting neutrons ( $\bar{v}=3.782$ in the case of ${ }_{98}^{252} C f$ ). In general, even-even nuclei have a strong tendency towards spontaneous fission:
${ }_{90}^{230} \mathrm{Th},{ }_{90}^{232} \mathrm{Th},{ }_{92}^{232} \mathrm{U},{ }_{92}^{234} \mathrm{U},{ }_{92}^{236} \mathrm{U},{ }_{92}^{238} \mathrm{U},{ }_{94}^{236} \mathrm{Pu},{ }_{94}^{238} \mathrm{Pu},{ }_{94}^{240} \mathrm{Pu},{ }_{94}^{242} \mathrm{Pu},{ }_{96}^{242} \mathrm{Cm}$,
${ }_{96}^{244} \mathrm{Cm},{ }_{96}^{246} \mathrm{Cm},{ }_{96}^{248} \mathrm{Cm}$
as do several odd-even pairs: ${ }_{92}^{235} \mathrm{U},{ }_{94}^{239} \mathrm{Pu},{ }_{95}^{241} \mathrm{Am}$
Spontaneous fission consists of disintegration regulated by a half-life like all forms of decay. It is often confused with induced fission brought about by neutron flux, although this reaction ceases in the absence of flux. Statistical studies have shown that the branching ratio of spontaneous fission decay of heavy isotopes with an even atomic number $Z$, and defined by:

$$
\lambda_{f s} \equiv B r \quad \lambda_{\text {total }}
$$

is empirically correlated by Y. Ronen's ratios ${ }^{39}$ as a function of the parameter $2 Z-N$ :

$$
\log _{10}(\mathrm{Br})=1,6247_{ \pm 0,0545} Z-1,03612_{ \pm 0,0687}(Z-N)-114,66_{ \pm 4,8}
$$

### 1.14 Radioactive Decay Branches

Radioactive decay chains are frequently depicted as series of boxes symbolizing isotopes. Logically, the tendency is to place the atomic mass number $A$ along the x -axis and the atomic number $Z$ along the y -axis (Fig. 1.32).

In our text, we shall use systematic shifting by one place for mass numbers between two rows of $Z$, which will enable us to show more developed decay chains on a single page. Indeed the physical predominance of neutron captures results in a

[^28]Fig. 1.32 Graphic representation of decays

tendency to "shift to the right", which simply means that the right-hand side of the page is rapidly reached. $\alpha$ radioactivity poses the same problem, but this time with movement towards the left. We will thus depict the isobaric decay chain for ${ }_{54}^{140} \mathrm{Xe}$ (Fig. 1.33). Some isotopes in fact have several competing modes of decay, meaning that disintegration of the isotope in question does not always have the same effect. In this case a statistical branching is defined that enables the modes of production to be quantified. The sum of these branching ratios is 1 .

$$
\begin{aligned}
& \sum_{\substack{\text { possible } \\
\text { decay } \\
\text { paths }}} \text { branching ratios }=1 \\
& \hline
\end{aligned}
$$

This phenomenon is clearly illustrated by the example of ${ }_{29}^{64} \mathrm{Cu}$, which follows $\beta^{-}, \beta^{+}$and electron capture (EC) decay modes. The Becquerel equation of ${ }_{29}^{64} \mathrm{Cu}$ is as follows:


Fig. 1.33 Decay chain of ${ }_{54}^{140} \mathrm{Xe}$

$$
\frac{d\left({ }_{29}^{64} C u\right)}{d t}=-\lambda_{29} C u\left({ }_{29}^{64} C u\right)
$$

That of ${ }_{30}^{64} \mathrm{Zn}$ shows $B r_{\beta^{-}}$branching, which indicates the proportion of $\beta^{-}$decay in the decay of ${ }_{29}^{64} \mathrm{Cu}$ (Fig. 1.34):

$$
\frac{d\left({ }_{30}^{64} \mathrm{Zn}\right)}{d t}=+B r_{\beta^{-}} \quad \lambda_{29} C u\left({ }_{29}^{64} \mathrm{Cu}\right)
$$

Meanwhile, the equation for ${ }_{28}^{64} N i$ is:

$$
\frac{d\left({ }_{28}^{64} N i\right)}{d t}=+B r_{\beta^{+}} \lambda_{29} C u\left({ }_{29}^{64} C u\right)+B r_{E C}{ }_{29}^{\lambda_{64} C u}\left({ }_{29}^{64} C u\right)
$$

The study of successive decay paths is a generalization of the problem for three isotopes (Bessis 1978, p. 39; Reine 1960, p. 73): radioactive isotope $N_{1}$ with a decay constant of $\lambda_{1}$, decays to $N_{2}$, itself radioactive, which itself decays with a decay constant of $\lambda_{2}$ to a stable isotope, $N_{3}$ (Mayo 1998, p. 182).

Fig. 1.34 Decay chain of ${ }_{29}^{64} \mathrm{Cu}$ which has several competing modes of decay


$$
N_{1} \xrightarrow{\lambda_{1}} N_{2} \xrightarrow{\lambda_{2}} N_{3} \text { stable. }
$$

Let us examine the activity $a_{i}(t)$ of these different isotopes under several hypotheses. The concentration of $N_{1}$ is given by:

$$
\frac{d N_{1}}{d t}=-\lambda_{1} N_{1}=-a_{1}(t) \quad \Rightarrow \quad N_{1}(t)=N_{1}^{0} e^{-\lambda_{1} t}
$$

That of $N_{2}$, according to the hypothesis of $N_{2}^{0}=0$, is given by:

$$
\left\{\begin{array}{l}
\frac{d N_{2}}{d t}=\lambda_{1} N_{1}-\lambda_{2} N_{2}=a_{1}(t)-a_{2}(t) \\
N_{2}(t)=\lambda_{1} N_{1}^{0}\left(\frac{e^{-\lambda_{1} t}-e^{-\lambda_{2} t}}{\lambda_{2}-\lambda_{1}}\right)
\end{array}\right.
$$

The activity $a_{1}(t)$ may be readily obtained from the previous expression:

$$
N_{2}(t)=\underbrace{\lambda_{1} N_{i}^{0} e^{-\lambda_{1} t}}_{a_{1}(t)} \quad \frac{\left(1-e^{-\left(\lambda_{2}-\lambda_{1}\right) t}\right)}{\lambda_{2}-\lambda_{1}}=\mathrm{a}_{1}(\mathrm{t}) \quad \frac{\left(1-\mathrm{e}^{-\left(\lambda_{2}-\lambda_{1}\right) \mathrm{t}}\right)}{\lambda_{2}-\lambda_{1}}
$$

Activity $a_{2}(t)$ is thus given by: $a_{2}(t)=\lambda_{2} \mathrm{a}_{1}(\mathrm{t}) \frac{\left(1-\mathrm{e}^{-\left(\lambda_{2}-\lambda_{1}\right) \mathrm{t}}\right)}{\lambda_{2}-\lambda_{1}}$
The concentration $N_{2}(t)$ is maximal where $d N_{2}(t) / d t=0$, i.e. where the two activities are equal, since $d N_{2}(t) / d t=a_{1}(t)-a_{2}(t)$, and thus where $\lambda_{2} \frac{\left(1-e^{-\left(\lambda_{2}-\lambda_{1}\right) t_{m}}\right)}{\lambda_{2}-\lambda_{1}}=1$, which leads to (Fig. 1.35):

Fig. 1.35 Activity of a parent isotope and of its radioactive daughter


Several scenarios may be imagined according to different values of $\lambda_{1}$ and $\lambda_{2}$. If $\lambda_{1}>\lambda_{2}$, the activities ratio may be simplified to:

$$
\frac{a_{2}(t)}{a_{1}(t)}=\frac{\lambda_{2} N_{2}(t)}{a_{1}}=\frac{\lambda_{2}}{\lambda_{1}-\lambda_{2}}\left(e^{\left(\lambda_{1}-\lambda_{2}\right) t}-1\right)
$$

which increases and tends towards infinity as time tends towards infinity. Where it is limited i.e. $\lambda_{1} \gg \lambda_{2}, e^{\left(\lambda_{1}-\lambda_{2}\right) t} \approx e^{\lambda_{1} t}$ and $\lambda_{2} /\left(\lambda_{1}-\lambda_{2}\right) \approx \lambda_{2} / \lambda_{1}$, activity $a_{2}(t)$ tends towards: $a_{2}(t) \approx \lambda_{2} N_{1}^{0} e^{-\lambda_{2} t}$.

Activity $a_{2}(t)$ quickly becomes independent of $a_{1}(t)$. Isotope $N_{1}$ rapidly gives way to its daughter isotope, and it may almost be said that $N_{2}$ is the head of an initial concentration chain $N_{1}^{0}$. This is known as chain reduction, and is the case with decay of ${ }_{52}^{131} T e$ :

$$
{ }_{52}^{131} \mathrm{Te} \quad{ }_{T_{1}}=\underset{1.25}{\overrightarrow{2}}{ }^{\text {days }}{ }_{53}^{131} I \underset{T_{2}=8}{ } \overrightarrow{\text { days }}{ }_{54}^{131} X
$$

However, where $\lambda_{1}<\lambda_{2}$, the activities ratio:

$$
\frac{a_{2}(t)}{a_{1}(t)}=\frac{\lambda_{2}}{\lambda_{2}-\lambda_{1}}\left(1-e^{-\left(\lambda_{2}-\lambda_{1}\right) t}\right)
$$

increases as $t \in\left[0, \lambda_{2} /\left(\lambda_{2}-\lambda_{1}\right)\right]$, and we speak of transient equilibrium.
In the extreme case in which $\lambda_{1} \ll \lambda_{2}$, the activities ratio tends towards $\lambda_{2} /\left(\lambda_{2}-\lambda_{1}\right)$ :

Fig. 1.36 Rapid decay of the head of a chain


$$
\frac{a_{2}(t)}{a_{1}(t)}=\frac{\lambda_{2}}{\lambda_{2}-\lambda_{1}}\left(1-e^{-\left(\lambda_{2}-\lambda_{1}\right) t}\right) \approx \frac{\lambda_{2}}{\lambda_{2}-\lambda_{1}}
$$

which will be very slightly greater than 1 . Here, we talk of secular equilibrium. As soon as an atom of $N_{2}$ appears, it decays immediately, and its activity is thus practically equivalent to that of its parent.

The decay chain of ${ }_{88}^{226} R a$ provides a perfect illustration of secular equilibrium: the activity of ${ }_{86}^{222} R n$ is practically equivalent to that of ${ }_{88}^{226} R a$.

$$
{ }_{88}^{226} R a \underset{ }{1600 \text { years }} \quad{ }_{86}^{222} R n \quad \underset{3.8 \text { days }}{\rightarrow} \quad{ }_{84}^{218} P o
$$

The special case of two isotopes $N_{1}$ and $N_{2}$ having the same half-lives, and thus the same decay constant, $\lambda$, is highly unlikely in reality. The generic solution given above cannot be applied in this case (division by $\left(\lambda_{2}-\lambda_{1}\right)$ is no longer possible). The solution for $N_{2}(t)$ may be obtained using the constant variation method (Figs. 1.36, 1.37 and 1.38):

$$
\begin{aligned}
& N_{2}(t)
\end{aligned}=C(t) e^{-\lambda t} .
$$

and : $\quad \frac{d N_{2}(t)}{d t}=-\lambda N_{2}+\lambda N_{1}=-\lambda C(t) e^{-\lambda t}+\lambda N_{1}^{0} e^{-\lambda t}$
giving: $\frac{d C(t)}{d t}=\lambda N_{1}^{0}$
By integration, we obtain: $C(t)=\lambda N_{1}^{0} t+B$. Constant $B$ may be found by $N_{2}(t)=$ $B=0$ hence:

Fig. 1.37 Daughter decays more rapidly than the parent


Fig. 1.38 Rapid decay of the daughter


$$
\begin{aligned}
& N_{1}(t)=N_{1}^{0} \quad e^{-\lambda t} \\
& N_{2}(t)=\lambda N_{1}^{0} t e^{-\lambda t} \\
& \frac{a_{2}(t)}{a_{1}(t)}=\frac{\lambda \lambda N_{1}^{0} t e^{-\lambda t}}{\lambda N_{1}^{0} \quad e^{-\lambda t}}=\lambda t
\end{aligned}
$$

### 1.15 Heavy Nucleus Chains

(Hyde et al. 1964; Joliot-Curie 1946)
All of the actinide decay chains may be grouped into four distinct chains (Fig. 1.39):

- The ${ }^{235} U{ }^{239} P u$ chain, which decays to stable lead-207 via successive $\alpha$ and $\beta$ decay, which are greatly accelerated after thorium-227.
- The ${ }^{233} U V^{241} P u$ chain, which decays to stable thallium-205 via successive $\alpha$ and $\beta$ decay, which are greatly accelerated after thorium-229. Bismuth-209, which occurs at the end of the chain, was considered stable until 2003 (at which point it

Fig. 1.39 Parent and daughter having the same half-life

was the only naturally-occurring stable isotope of bismuth), when a French team detected its $\alpha$ radioactivity ${ }^{40}$ and successfully determined its extremely long half-life ( $T=1.9_{ \pm 0.2} \quad 10^{19}$ years). By comparison, the estimated age of the universe is 13.7 billion years based on the Hubble constant, $H_{0}=75 \mathrm{~km} / \mathrm{s} /$ Mpar sec.

- The ${ }^{238} U /^{242} P u$ chain, which decays to stable lead-206 via successive $\alpha$ and $\beta$ decay, which are greatly accelerated after radon-222, despite the fact that relatively long-lived lead-210 occurs between the rapid isotopes.
- The ${ }^{236} U /^{240} P u$ chain, which decays to stable lead-208 via successive $\alpha$ and $\beta$ decay, which are greatly accelerated after thorium- 228 .

This chain comprises in particular the sub-chain ${ }_{92}^{239} U \rightarrow{ }_{93}^{239} \mathrm{~Np} \rightarrow{ }_{94}^{239} \mathrm{Pu}$, which is the main mode of formation in reactors and plays an important role in the residual power present for a short period following reactor shutdown (Fig. 1.40).

This chain comprises in particular the sub-chain ${ }_{94}^{241} \mathrm{Pu} \rightarrow{ }_{95}^{241} \mathrm{Am}$, which diminishes the quality of stocked plutonium (Figs. 1.41, 1.42 and 1.43).

[^29]$$
\text { Fig. 1.40 The }{ }_{92}^{235} \mathrm{U} /{ }_{94}^{239} P u \text { chain, terminating with }{ }_{82}^{207} \mathrm{~Pb}
$$
\[

$$
\begin{aligned}
& \text { Infographie Marguet }
\end{aligned}
$$
\]

$$
\begin{aligned}
& \begin{array}{l}
1.78 \mathrm{lo}^{-3} \mathrm{~s} \\
{ }_{84}^{215} \mathrm{Po} \\
2.17 \mathrm{~min}
\end{array} \\
& 4
\end{aligned}
$$

$$
\begin{aligned}
& \uparrow \\
& \begin{array}{l} 
\\
\\
\\
\\
\\
\\
{ }_{88}^{223} R a \\
11.43 \mathrm{~d}
\end{array}
\end{aligned}
$$


Fig. 1.41 The ${ }_{92}^{233} U /{ }_{94}^{241} P u$ chain, terminating with ${ }_{81}^{205} T l$
Infographie Marguet
$\longrightarrow{ }_{86}^{3.8 \mathrm{~d}} \mathrm{Rn} \longrightarrow{ }_{84}^{2.05 \mathrm{~min}} \mathrm{PO}_{8}^{218} \longrightarrow{ }_{82}^{214} \mathrm{~Pb}$

Fig. 1.42 The ${ }_{92}^{238} \mathrm{U} /{ }_{94}^{242} \mathrm{Pu}$ chain, terminating with ${ }_{82}^{206} \mathrm{~Pb}$

Fig. 1.43 The ${ }_{92}^{236} U /{ }_{94}^{240} \mathrm{Pu}$ chain, terminating with ${ }_{82}^{208} \mathrm{~Pb}$

# Chapter 2 <br> Interaction Between Neutrons and Matter 

Studying the behavior of neutrons in a reactor enables us to understand how fission phenomena occur and how they may be controlled in a power reactor. The science of neutrons, or neutron physics, is greatly indebted to Enrico Fermi, who contributed extensively to the mathematics in this field thanks to his initial mathematical training. The relatively slow speed of neutrons in reactors nevertheless means that no relativistic effects need to be taken into account, which greatly simplifies calculations. However, this speed is not always sufficiently rapid to allow the intrinsic speed of target atoms to be overlooked due to the temperature. In this context, the notion of reference frameworks (laboratory or center of mass) is thus capital.

### 2.1 Neutron Scattering

(Egelstaff 1965; Egelstaff and Poole 1969)
Neutron scattering ${ }^{1}$ in the core of a nuclear reactor is of central importance to an understanding of reactor physics. The word scattering is frequently found in different sciences, particularly in thermics and in chemistry, and refers to the same physical phenomenon, namely the collision between two atoms or, in our case, the collision between a neutron and an atomic nucleus. We can first of all carry out a didactic analysis of the collision between neutrons and matter by comparing it with the collision between two "balls" of different (or equivalent) size. Those who play pool thus have a very practical grasp of the notion of scattering. Scattering is said to be elastic when kinetic energy is preserved, in other words, the objects involved in the collision retain their fundamental state. Scattering is termed inelastic if at least one of the objects involved undergoes excitation, with removal of

[^30]energy from the kinetic energy balance (in concrete terms, there is no longer conservation of kinetic energy before and after the collision). The elastic scattering of spin nucleons by nuclei comes under the general theory of quantum physics of Wolfenstein and Ashkin ${ }^{2}$, which is too complex to be adequately dealt with here (see Progress in Nuclear Physics Vol 8 1960b, p49), and the mathematical aspects of which are dealt with in Lax and Phillips (1967). For the present purposes, we shall simply analyze elastic scattering by means of calculation using the Newtonian formulation of speeds before and after the collision of impenetrable particles. The notion of frameworks is of fundamental importance in this setting. It is important to clearly distinguish the laboratory framework, which is of capital interest to the observer, who is generally associated with the laboratory, and in which reactor physics calculations are carried out, from the center-of-mass framework, which enables certain physical calculations to be simplified.

### 2.1.1 Elastic Scattering on a Fixed Target

(Delcroix 1959, p1; Mayo 1998, p95; Meghreblian and Holmes 1960, p69)
We will therefore study elastic scattering as a phenomenon identical to the collision between two pool balls in Newtonian mechanics, with the difference being that in general, neutrons have a far lower mass than their target, except where the target is a hydrogen nucleus comprising a proton of much the same mass as that of a neutron. We will begin (we shall see the second phase of this reasoning in Chap. 7) by assuming that speed of a neutron projectile is extremely high compared to the thermal agitation of the nucleus taken as a fixed target. The hypothesis of inelastic scattering is based on the notion that the energy of a neutron does not in theory exceed the excitation energy of the first excited state energy level of the target atom. This energy may have very different thresholds depending on target, ranging from several tens of keV for relatively heavy nuclei such as uranium to several MeV for light nuclei. Inside a reactor, no neutrons produced from fission have an energy greater than 14 MeV and the experimental mean of the fission spectrum is 2 MeV .

In quantitative terms, elastic scattering thus represents the largest number of collisions within the reactor, as we shall see below. In the laboratory framework, a neutron of speed $v$ collides with a nucleus of atomic mass $M$, which is considered as being initially immobile. The speeds after collision are denoted by ' (prime). In the center-of-mass framework in which speeds are denoted by $\otimes$, the neutron and target approach the center of mass where they will collide (Figs. 2.1, 2.2 and 2.3). The physical laws of collision involved the real masses of particles. In the laboratory framework, the very definition of the center of mass, $G$, is given by the vectorial relationship $(M+m) \overrightarrow{O G} \equiv m \overrightarrow{O n}+M \overrightarrow{O N}$, which is derived in relation to time:

[^31]

Fig. 2.1 Elastic scattering


Fig. 2.2 Elastic scattering at the laboratory frame


Before scattering


After scattering

Fig. 2.3 Elastic scattering on fixed target at center of mass frame (speeds are marked $\otimes$ )

$$
(M+m) \frac{d \overrightarrow{O G}}{d t}=m \underbrace{\frac{d \overrightarrow{O n}}{d t}}_{\vec{v}}+M \underbrace{\frac{d \overrightarrow{O N}}{d t}}_{\overrightarrow{0}}
$$

before the collision in the laboratory frame. Since the target is fixed, the vector $\overrightarrow{O N}$ does not vary with time; its temporal derivative is nil. Through the definition of the speed of the neutron at position $n$, we have $\vec{v}=d \overrightarrow{O n} / d t$.

$$
\text { Giving: } \quad \vec{v}_{\substack{G \text { before } \\ \text { collision }}}=\frac{d \overrightarrow{O G}}{d t}=\frac{m}{(M+m)} \vec{v}
$$

In the frame of reference of the center of gravity, $\overrightarrow{V_{\otimes}}=\frac{d \overrightarrow{G N}}{d t}=-\frac{m}{(M+m)} \vec{v}$ before collision since:

$$
\left\{\begin{array}{l}
\overrightarrow{O N}=\overrightarrow{O G}+\overrightarrow{G N} \\
\overrightarrow{0}=\frac{d \overrightarrow{O G}}{d t}+\frac{d \overrightarrow{G N}}{d t} \quad \text { and } \quad \frac{d \overrightarrow{O G}}{d t}=\frac{m}{(M+m)} \vec{v}
\end{array}\right.
$$

Similarly, $\vec{v}_{\otimes}=\frac{d \overrightarrow{G n}}{d t}=\frac{M}{M+m} \vec{v}$ before collision since:

$$
\left\{\begin{array}{l}
\overrightarrow{O n}=\overrightarrow{O G}+\overrightarrow{G n} \\
\frac{d \overrightarrow{O n}}{d t}=\frac{d \overrightarrow{O G}}{d t}+\frac{d \overrightarrow{G n}}{d t} \Rightarrow \vec{v}=\frac{m}{M+m} \vec{v}+\frac{d \overrightarrow{G n}}{d t}
\end{array}\right.
$$

The conservation of kinetic energy at the center of mass frame (the hypothesis on which elastic scattering is based) is given by:
$\frac{1}{2} M \underbrace{\left(\frac{m v}{M+m}\right)^{2}}_{V_{\otimes}}+\frac{1}{2} m \underbrace{\left(\frac{M v}{M+m}\right)^{2}}_{v_{\otimes}}=\frac{1}{2} m v_{\otimes}^{\prime 2}+\frac{1}{2} M V_{\otimes}^{\prime 2}$ at the center of mass frame
At the center of mass frame, $m \vec{v}_{\otimes}^{\prime}+M \vec{V}_{\otimes}^{\prime}=\overrightarrow{0}=(M+m) \underbrace{\vec{v}_{G \otimes}^{\prime}} \Rightarrow v_{\otimes}^{\prime}=\frac{M}{m} V_{\otimes}^{\prime}$
0 by
definition
Since the impulse is nil, this means that the speeds are opposite and collinear and of modules inversely proportional to the masses.

$$
\text { Hence: }\left\{\begin{array}{l}
v_{\otimes}=\frac{M}{M+m} v=v_{\otimes}^{\prime} \\
V_{\otimes}=\frac{m}{M+m} v=V_{\otimes}^{\prime}
\end{array}\right.
$$

It should be noted that there is no variation in speed at the center of mass frame. This is a highly specific characteristic of elastic scattering in the center of mass frame, the importance of which is now apparent. Note also that at the laboratory frame, neutron speed decreases by a factor of $M /(M+m)$, which varies inversely with $M$. The speed at the center of mass $G$ is nil before and after scattering at the center of mass. Another value is also of great importance in characterizing scattering, namely the angle $\theta$ between the direction of travel of the scattered neutron and its initial trajectory in the laboratory frame, which enables us to answer the
fundamental question: In which direction does a neutron travel following collision? The answer to this question allows increasingly precise of the complete trajectory of the neutron in deterministic fashion. Conservation of the momentum $\vec{p}$ before and after scattering in the laboratory framework is expressed as:


Furthermore, $(M+m) \overrightarrow{\mathrm{v}}_{\mathrm{G}}^{\prime}=m \vec{v}^{\prime}+M \vec{V}^{\prime}$ by definition of the center of gravity, hence:

$$
\vec{v}_{G}^{\prime}=\frac{d \overrightarrow{O G}}{d t}=\frac{m}{(M+m)} \vec{v}=\vec{v}_{G}
$$

The speed of the center of mass in the laboratory framework is constant before and after scattering. The composition of the speeds in the two frameworks is given by:
before scattering

$$
\begin{aligned}
& \frac{d \overrightarrow{O n}}{d t}=\frac{d \overrightarrow{O G}}{d t}+\frac{d \overrightarrow{G n}}{d t} \\
& \downarrow \\
& \vec{v}=\frac{\downarrow}{M+m}+\frac{M \vec{v}}{M+m} \\
& \vec{v}^{\prime}=\frac{m \vec{v}}{M+m}+\vec{v}_{\otimes}^{\prime}
\end{aligned}
$$

Projecting onto 0x (Fig. 2.4):

$$
v^{\prime} \cos \theta=\frac{m}{M+m} v+v_{\otimes}^{\prime} \cos \Psi
$$

where $v_{\otimes}^{\prime}=\frac{M}{M+m} v$

$$
v^{\prime 2}=\left(\frac{m}{M+m} v\right)^{2}+2 \cos \psi \frac{m}{M+m} v v_{\otimes}^{\prime}+v_{\otimes}^{\prime 2}
$$

Substituting $v_{\otimes}^{\prime}$, we get: $v^{\prime 2}=\left(\frac{M^{2}+2 M m \cos \psi+m^{2}}{(M+m)^{2}}\right) v^{2}$


Fig. 2.4 Velocity triangle (fixed target)

Where:

$$
\left\{\begin{array}{l}
v^{\prime} \cos \theta=\left(\frac{m+M \cos \psi}{M+m}\right) v \\
v^{\prime 2}=\left(\frac{M^{2}+2 M m \cos \psi+m^{2}}{(M+m)^{2}}\right) v^{2}
\end{array}\right.
$$

$$
\cos \theta=\frac{m+M \cos \psi}{\sqrt{M^{2}+2 M m \cos \psi+m^{2}}}
$$

is the cosine of the scattering angle in the laboratory framework (Fig. 2.4).
At this stage of the calculation, even though we are nearer to identifying the angle (via its cosine), we can see that it depends on $\mu_{0}=\cos \psi$, a value shown in the diagram of speeds after scattering in the center-of-mass frame. We thus have no absolute knowledge of the scattering angle of the neutron, which is a concrete example of the difficulty in determining exactly where a pool ball will land after a collision! However, a key hypothesis that will enable us to progress is as follows: if there are no directions of predilection for scattering, in other words scattering is isotropic at the center of mass frame of a fixed target, the probability of scattering at the solid angle $d \Omega$ is $d \Omega / 4 \pi$. If scattering occurred consistently in the same plane, there would be an equal probability of angle $\psi$ assuming any value between $0^{\circ}$ and $180^{\circ}$. However, since the scattering plane is not fixed, the cosine of angle $\psi$ is equiprobable between $[-1,+1]$, which, in other words, predicts that the neutron may be scattered anywhere within the $4 \pi$ steradians of space around the collision in the center-of-mass framework. In practice, this hypothesis has been amply verified for light target nuclei and for energies below 1 MeV . The geometrical symmetry of the nucleus also affects the isotropism of scattering. The mean value of $\cos \theta$, very commonly noted $\bar{\mu}$, may also be calculated using the following hypothesis as follows (Meghreblian and Holmes 1960, p78):

$$
\begin{aligned}
\overline{\cos \theta}= & \frac{\int_{0}^{4 \pi} \frac{m+M \cos \psi}{\sqrt{M^{2}+2 M m \cos \psi+m^{2}}} d \Omega}{\int_{0}^{4 \pi} d \Omega}=\frac{\int_{0}^{\pi} \frac{m+M \cos \Psi}{\sqrt{M^{2}+2 M m \cos \Psi+m^{2}}} 2 \pi \sin \Psi d \Psi}{\int_{0}^{4 \pi} d \Omega=4 \pi} \\
\overline{\cos \theta} & =\frac{1}{2} \int_{-1}^{+1} \frac{m+M x}{\sqrt{M^{2}+2 M m x+m^{2}}} d x \\
& =\frac{1}{2}(\underbrace{m \frac{1}{M m}\left[\sqrt{M^{2}+2 M m x+m^{2}}\right]_{-1}^{+1}}_{\frac{2 m}{M}}+\underbrace{\int_{-1}^{+1} \frac{M x}{\sqrt{M^{2}+2 M m x+m^{2}}} d x}_{-\frac{2}{3} \frac{m}{M}})
\end{aligned}
$$

Ultimately,
Mean cosine of scattering angle in laboratory framework: $\overline{\cos \theta}=\frac{2}{3} \frac{m}{M}$
where $M$ is the mass of the target, $m$ is the mass of the neutron, and $\theta$ is the scattering angle of the neutron in the laboratory framework.

The mean energy after scattering may be calculated as follows:

$$
\begin{aligned}
\overline{E^{\prime}} & \left.=\frac{1}{2} m \overline{v^{\prime 2}}=\frac{1}{2} m \frac{\int_{0}^{\pi}\left(\frac{M^{2}+2 M m \cos \psi+m^{2}}{(M+m)^{2}}\right) v^{2} 2 \pi \sin \psi d \psi}{4 \pi}\right]_{0}^{(M+m)^{2}} \\
& =\frac{1}{2} m v^{2}\left[\frac{-M^{2} \cos \psi+M m \sin ^{2} \psi-m^{2} \cos \psi}{(M+m)^{2}}\right. \\
& =E \frac{M^{2}+m^{2}}{(M+1}
\end{aligned}
$$

These results, which are particularly simple, are only valid for isotropic scattering in the center of mass frame and the fixed target. They are thus not valid as regards thermal energy in particular, since the speed of the neutron becomes practically equal to that of the agitation of its target. This result is frequently presented in reference works in the form $\overline{\cos \theta}=2 /(3 A)$, where $A$ is the mass number of the target (GA Vol. 1 1967, p209). This comes from a shortcut in writing the equations, in which the mass of the neutron is taken as one unit of atomic mass (in reality, $1.008 u$ ) and the target is taken as having a mass of $A$ units of atomic mass. This is tantamount to replacing $m$ by 1 and $M$ by $A$ in all the foregoing formulae. These approximations are conventionally acceptable to within $1 \%$. This result shows that scattering is in fact not at all isotropic in the laboratory framework. The mean value of angle $\theta$ in fact tends towards $90^{\circ}$ as the mass number increases, and for lower mass numbers, scattering occurs in the forward direction. Note the
special case in which the mass of the target is equal to the mass of the incident particle. The formula $\cos \theta$ gives an indeterminate form when $\Psi=\pi$, which can be resolved using l'Hôpital's rule on the limit of a quotient:

$$
\begin{aligned}
\lim _{\cos \Psi \rightarrow-1}\left(\frac{m+m \cos \Psi}{\sqrt{m^{2}+2 m^{2} \cos \Psi+m^{2}}}\right) & =\left(\frac{\frac{d(m+m x)}{d x}}{\frac{d \sqrt{m^{2}+2 m^{2} x+m^{2}}}{d x}}\right)_{-1} \\
& =\left(\frac{\sqrt{m^{2}+2 m^{2} x+m^{2}}}{m}\right)_{-1}=0
\end{aligned}
$$

This result shows that angle $\theta$ tends towards $\pi / 2$. Where the masses are strictly identical, the incident particle may be stopped dead with transmission of all its energy to the target. Curiously, if mass $m$ diverges from $M$ (even very slightly, as in the case of a proton and a neutron), for $\cos \Psi=-1$, we have:

$$
\cos \theta=\frac{m-M}{\sqrt{M^{2}-2 M m+m^{2}}}=\left\{\begin{aligned}
1 & \text { if } m>M \\
-1 & \text { if } m<M
\end{aligned}\right.
$$

Regarding the target nucleus, the cosine of angle $\varphi$ cannot be negative, meaning that the nucleus is consistently ejected in the forward direction (Berthelot 1956, p14). It may also be seen that, disregarding the absorption problems of neutrons, heavy materials have a greater reflective potential per atom (greater backscattering) with regard to neutron scattering. However, this remark must be tempered by the fact that the greater the mass number of the target, the less effective will be the slowing down of neutrons, as we saw in our presentation of scattering laws (Table 2.1).

Angle $\overline{\bar{\theta}}=\operatorname{Arc} \cos (\overline{\cos \theta})$, which is in fact devoid of any physical meaning, is only of value in demonstrating that this mean pseudo-angle rapidly tends towards $90^{\circ}$ as the target mass number increases. Generally speaking, it is fairly standard to consider scattering as isotropic at the center of mass. We know that inelastic scattering is generally isotropic up to an energy of 1 MeV . With inelastic scattering, this threshold falls to around 100 keV , thus seriously challenging the very widely held belief that elastic scattering is always isotropic. In general, elastic scattering tends to be mostly in a forward direction as the energy of the incident neutron increases.

Table 2.1 Mean neutron deflection by target mass

| Atom | ${ }_{1}^{1} H$ | ${ }_{1}^{2} D$ | ${ }_{4}^{9} B e$ | ${ }_{6}^{12} C$ | ${ }_{92}^{238} U$ |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $A$ | 1 | 2 | 9 | 12 | 238 | $\infty$ |
| $\overline{\cos \theta}$ | 0.667 | 0.333 | 0.074 | 0.056 | 0.0028 | 0 |
| $A r c \cos (\overline{\cos \theta})$ | $48^{\circ}$ | $70.5^{\circ}$ | $86^{\circ}$ | $87^{\circ}$ | $89.8^{\circ}$ | $90^{\circ}$ |

### 2.1.2 Elastic Scattering on a Moving Target

A key assumption in the foregoing calculations is that the target is completely immobile. The use of neutrons as a means of investigating matter has resulted in a great deal of theoretical work on the quasi-elastic interaction between neutrons and both solids and liquids (Springer 1972). Within the bounds of reactor physics, the atoms that make up the materials involved are subject to thermal agitation. We shall examine this subject in greater detail in the chapter dealing with the Doppler effect. In the present section, we shall simply examine the implications of the speed of the target on the foregoing formulae. We saw that elastic scattering thus consists of simple rotation of velocity vectors in the center of mass. If the target is mobile, the speed triangle is modified as a result of speed $\vec{V}$ of the target prior to scattering: $\theta$ is the scattering angle in the laboratory framework (between $\vec{v}_{G}$ and $\overrightarrow{v^{\prime}}$ ), and $\psi$ is the scattering angle in the center-of-mass framework (Fig. 2.5).

It is important to note that angle $\theta$, and thus its cosine, $\mu=\cos \theta$, are not independent of velocity $v$. All points $P$ describing the entire sphere of radius $v^{\prime}$ may be reached with equal probability if the collision is isotropic in the center of mass. The speed of the center of mass is given by:

$$
\vec{v}_{G}^{\prime}=\frac{d \overrightarrow{O G}}{d t}=\frac{m}{(M+m)} \vec{v}+\frac{M}{(M+m)} \vec{V}=\vec{v}_{G}
$$

Hence: $v_{G}^{2}=\frac{m^{2} v^{2}+2 m M v V \cos \varphi+M^{2} V^{2}}{(M+m)^{2}}$ where $\varphi$ is the angle between $\vec{V}$ and $\vec{v}$
If $A=\frac{M}{m}$ and $v_{G}^{2}=\frac{v^{2}+2 A v V \cos \varphi+A^{2} V^{2}}{(A+1)^{2}}$, the relative velocity of the neutron in relation to the target is given by:

Fig. 2.5 Velocity triangle (moving target)


$$
\vec{v}_{r}=\vec{v}-\vec{V} \quad \text { with } \quad v_{r}^{2}=v^{2}+V^{2}-2 v V \cos \varphi
$$

further: $\vec{v}_{\otimes}=\frac{A}{A+1} \vec{v}_{r}, \quad$ hence $\quad v_{\otimes}^{\prime}=v_{\otimes}=\frac{A}{A+1} v_{r}$
Since: $\quad \overrightarrow{v^{\prime}}=\vec{v}_{G}+\vec{v}_{\otimes}^{\prime}$, we have: $\quad v_{\otimes}^{\prime 2}=v_{G}^{2} \sin ^{2} \theta+\left(v^{\prime}-v_{G} \cos \theta\right)^{2}$
And $\quad v^{\prime 2}=v_{G}^{2}+v_{\otimes}^{\prime 2}+v_{G} v_{\otimes}^{\prime} \cos \psi$ with $v_{\otimes}^{\prime}=v_{\otimes}^{\prime}=\frac{A}{A+1} v_{r}$
Hence: $\quad \cos \theta=\frac{v_{G}^{2}+v^{\prime 2}-\frac{A^{2}}{(A+1)^{2}} v_{r}^{2}}{2 v_{G} \nu^{\prime}}$
Regarding angle $\psi$, the isotropic scattering means that $\cos \psi$ varies equiprobably between -1 and 1 , and the probability density is thus $1 / 2$ for $[-1,+1]$ and 0 elsewhere. In reality, the collision is not isotropic in the center of mass, particularly at low energies, where the chemical bond energy of atoms in molecules becomes considerable in relation to the energy of the neutron, and at high energies, where forward scattering becomes very marked. Overall, forward scattering is very slightly anisotropic. This may be represented by a probability density biased towards forward scattering with $\mu=\cos \theta$ and $\mu_{0}=\cos \psi$ according to the following formula:

$$
p\left(\mu_{0}\right) d \mu_{0}=\frac{1}{2}\left(1+3 \overline{\mu_{0}} \mu_{0}\right) d \mu_{0}
$$

for which the mean value is $\int_{-1}^{+1} p\left(\mu_{0}\right) \mu_{0} d \mu_{0}=\left[\frac{1}{2}\left(\frac{\mu_{0}^{2}}{2}+3 \overline{\mu_{0}} \frac{\mu_{0}^{3}}{3}\right)\right]_{-1}^{+1}=\overline{\mu_{0}}$
$\overline{\mu_{0}}$ is the mean value of the cosine of the scattering angle in the center-of-mass framework, the theory of which enables an approximated value to be calculated as a function of total energy:

$$
E=\frac{1}{2} \frac{m M}{m+M} v_{r}^{2}=\frac{1}{2} \frac{m A}{A+1} v_{r}^{2} \quad \overline{\mu_{0}} \approx 0.07 A^{\frac{2}{3}} E_{[\mathrm{MeV}]}
$$

Allowing for this anisotropy in the calculation of $\bar{\mu}$ leads to a correction (Woods 1964) of the previous calculation $(\bar{\mu}=2 /(3 A))$ that is valid when the temperature of the moderator is low (and thus the speed of the target is low comparatively with that of the neutron) and of the form:

$$
\bar{\mu}=\frac{2}{3 A}+\bar{\mu}_{0}\left(1-\frac{3}{5 A^{2}}\right)
$$

Note that the degree of isotropy of scattering at the center of the laboratory augments as the mass of the target increases.

### 2.1.3 Moderator

The neutron emitted at energy $E_{0}=m v_{0}^{2} / 2$, i.e. around 2 MeV in the case of fission, may be slowed down in a thermal reactor to an energy of around $E_{n}=0.0253 \mathrm{eV}(300 \mathrm{~K}, 2200 \mathrm{~m} / \mathrm{s})$.

$$
E_{1}=\frac{1}{2} m v_{1}^{2}=\frac{1}{2} m \frac{M^{2}+2 M m \cos \psi+m^{2}}{(M+m)^{2}} v_{0}^{2}=\frac{M^{2}+2 M m \cos \psi+m^{2}}{(M+m)^{2}} E_{0}
$$

Energy $E_{1}$ is a random variable due to the presence of $\cos \psi$. The term 2 Mm $\cos \psi$ before $M^{2}+m^{2}$ may be reasonably overlooked (which is equivalent to considering a right-angle collision), and calculating the successive energy after $n$ collisions, we obtain:

$$
E_{\text {ncollisions }} \approx\left(\frac{M^{2}+m^{2}}{(M+m)^{2}}\right)^{\mathrm{n}} E_{0} \quad \text { Thus: } n=\frac{\ln \left(\frac{E_{0}}{E_{n}}\right)}{2 \times \ln (M+m)-\ln \left(M^{2}+m^{2}\right)}
$$

It is now possible to calculate the approximate value of $n$ that enables us to obtain the thermal energy $E_{n}=0.0253 \mathrm{eV}$. The following table shows the percentage energy loss at the first collision as well as the approximate number of collisions required to reach thermal energy (Table 2.2):

Obviously, this result is only an indication given the highly simplified hypotheses on which it is based, namely considering the collisions as right angles. Reuss (2004, p190) correctly notes that the previous reasoning leads to multiplication of the energy ratios before and after scattering. Each ratio is a random variable, and the statistical mean of a product is not equivalent to the product of the means. A logarithmic approach, which we shall follow in Chap. 4 below, is accurate to the extent that it sums logarithmic increments and that the mean of the sum is rightly in this case the sum of means. Nonetheless, we may conclude that from the strict standpoint of scattering, light nuclei are superior to heavy nuclei in terms of slowing down power. Although capture by the latter is negligible, they will thus make good moderators, and the aim of the reactor physician is to continually seek to optimize neutron loss in order to ensure effective fuel use. Similarly, a good moderator will take the densest chemical form possible in order to increase the number of atoms of moderator per unit volume, which in turn will result in more effective slowing down of neutrons. Liquid water presents a good technical compromise in terms of density/ low absorption/low mass number, and is also a useful option for thermal spectrum reactors.

Table 2.2 Energy loss of neutrons by target mass

|  | ${ }_{1}^{1} \mathrm{H}$ | ${ }_{1}^{2} \mathrm{H}$ | ${ }_{6}^{12} \mathrm{C}$ | ${ }_{8}^{16} \mathrm{O}$ | ${ }_{11}^{23} \mathrm{Na}$ | ${ }_{92}^{238} \mathrm{U}$ |
| :--- | :--- | :--- | ---: | ---: | ---: | :--- |
| $\left(E_{0}-E_{1}\right) / E_{0} \%$ | 50 | 44 | 14 | 11 | 8 | 0.8 |
| $n$ | 27 | 31 | 121 | 157 | 222 | 2200 |

### 2.1.4 Inelastic Scattering

Inelastic scattering is characterized by the non-conservation of kinetic energy before and after collision. Some of the energy of the incident particle may be absorbed by the target nucleus, which is then in an excited state. This reaction can only occur if the kinetic energy of the incident neutron is greater than the difference in energy between the first level of excitation of the nucleus and the ground state. Hence inelastic scattering is a threshold reaction. The neutron is then re-emitted and carries with it the residual energy not expended in excitation of the target nucleus.

$$
{ }_{0}^{1} n+{ }_{3}^{7} L i \rightarrow{ }_{3}^{7} L i^{*}+{ }_{0}^{1} n \quad * \text { denotes that the nucleus is excited }
$$

If the incident particle is a neutron, we speak of $\left(n, n^{\prime}\right)$ scattering, with $n^{\prime}$ indicating that the re-emitted neutron does not have the same characteristics as the incident neutron (which may be a different neutron in fact). Using this notation, it is possible to distinguish between inelastic scattering and elastic scattering. Total energy conservation is written as:

Total energy conservation in the center of mass:

$$
\begin{equation*}
\frac{1}{2} m v_{\otimes}^{2}+\frac{1}{2} M V_{\otimes}^{2}+m c^{2}+M c^{2}=\frac{1}{2} m v_{\otimes}^{\prime 2}+\frac{1}{2} M^{*} V_{\otimes}^{\prime 2}+m c^{2}+M^{*} c^{2} \tag{2.2}
\end{equation*}
$$

Here, an asterisk indicates the mass of the excited target, $M^{*}$. Using $Q$ to denote the excitation energy of the first nuclear level, we may state that:

$$
M^{*}=M+\frac{Q}{c^{2}}
$$

Since the kinetic energy is generally low in relation to the rest energy, we normally write:

$$
\frac{1}{2} M^{*} V_{\otimes}^{\prime 2} \approx \frac{1}{2} M V_{\otimes}^{\prime 2}
$$

The balance is thus:

$$
\frac{1}{2} m v_{\otimes}^{2}+\frac{1}{2} M V_{\otimes}^{2}=\frac{1}{2} m v_{\otimes}^{\prime 2}+\frac{1}{2} M V_{\otimes}^{\prime 2}+Q
$$

This formula may be used to calculate the threshold kinetic energy in the laboratory framework needed to excite the target nucleus. It corresponds to the kinetic energy of a neutron with zero scattering in the center of mass, in the same way as the kinetic energy of the target nucleus after collision. We thus find that:

$$
\frac{1}{2} m v_{\otimes}^{2}+\frac{1}{2} M V_{\otimes}^{2}=\frac{1}{2} \frac{m M}{m+M} v^{2}=\frac{M}{m+M} E_{\text {threshold }}=Q
$$

If the kinetic energy of the neutron (laboratory framework) is below this threshold, only elastic scattering is possible. If it is above this threshold, elastic scattering and inelastic scattering compete, and the higher the energy the greater the inelastic scattering will be. The formula shows that the threshold is lower as the target mass decreases. Inelastic scattering modifies both the kinetic energy of the scattered neutrons and their scattering angle. Since the amount of movement remains zero before and after collision in the center of mass, the following continues to apply:

$$
\begin{gathered}
M^{*} \overrightarrow{V_{\otimes}^{\prime}}+m \overrightarrow{v_{\otimes}^{\prime}}=0 \\
\text { Hence: }\left\{\begin{array}{l}
v_{\otimes}^{\prime} 2=\left(\frac{m}{m+M}\right)^{2} v^{2} \tilde{A}^{2}(E) \\
\tilde{A}(E)=\frac{M}{m} \sqrt{1-\frac{m+M}{M} \frac{Q}{E}}=\frac{M}{m} \sqrt{1-\frac{E_{\text {threshold }}}{E}}
\end{array}\right.
\end{gathered}
$$

The energy of the scattered neutron in the laboratory framework may be written as follows, assuming that $A=M / m$ :
$E^{\prime}=\frac{\left(1+\widetilde{A}^{2}(E)+2 \widetilde{A}(E) \cos \Psi\right)}{(A+1)^{2}} E \quad$ and also: $\quad v^{\prime 2}=\frac{\left(1+\widetilde{A}^{2}(E)+2 \widetilde{A}(E) \cos \Psi\right)}{(A+1)^{2}} v^{2}$
At the laboratory frame, the neutron is deflected at angle $\theta$ such that:
Deflection by inelastic scattering: $\begin{aligned} \cos \theta & =\frac{\left(1+\widetilde{A}(E) \mu_{0}\right)}{A+1} \frac{v}{v^{\prime}} \\ & =\frac{1+\widetilde{A}(E) \mu_{0}}{\sqrt{1+\widetilde{A}^{2}(E)+2 \widetilde{A}(E) \mu_{0}}}\end{aligned}$
This formula, in which $E$ is the energy before collision, is also valid for elastic scattering where $\tilde{A}(E)=A$. Within a certain energy domain, it is no longer possible to distinguish between the different levels of excitation, and we speak of the unresolved range. The probability of slowing down of energy is modeled using a continuous function, occasionally referred to as the evaporation spectrum, as follows ${ }^{3}$ (Price et al. 1957, p121):

[^32]$$
p\left(E^{\prime} \rightarrow E\right)=\frac{E}{I} e^{-\frac{E}{\theta\left(E^{\prime}\right)}}
$$
where $I$ is a normalization constant and $\theta\left(E^{\prime}\right)$ is a tabulation dependent on the energy of the incident neutron. If the energies of the inelastic excitation levels are known, which shall be denoted as $E_{i}$ with $i$ being the index of the excitation level, the inelastic cross-section is written as:
$$
\sigma_{s}^{i}\left(E^{\prime} \rightarrow E\right)=\sigma_{s}^{i}\left(E^{\prime}\right) p_{i}\left(E^{\prime}, \mu_{0}\left(E^{\prime}, E\right)\right) \frac{d \mu_{0}\left(E^{\prime}, E\right)}{d E}
$$
where:

- $\sigma_{s}^{i}\left(E^{\prime}\right)$ is the cross-section corresponding to the energy level, integrated in the incident energy,
- $p_{i}\left(E^{\prime}, \mu_{0}\left(E^{\prime}, E\right)\right)$ is the probability of angular scattering,
- $\mu_{0}(E, E)=\cos \Psi$ is the cosine of the scattering angle in the center of mass.

In accordance with what was seen earlier:

$$
\mu_{0}\left(E^{\prime}, E\right)=\frac{\frac{(A+1)^{2}}{2 A} \frac{E}{E^{\prime}}+\frac{A}{2} \frac{E_{i}}{E}-\frac{A^{2}+1}{2 A}}{\sqrt{1-\frac{E_{i}}{E^{\prime}}}}=\frac{(A+1)^{2} \frac{E}{E^{\prime}}-\left(1+\widetilde{A}^{2}\left(E^{\prime}\right)\right)}{2 \widetilde{A}\left(E^{\prime}\right)}
$$

where $\widetilde{A}\left(E^{\prime}\right)=A \sqrt{1-E_{i} / E^{\prime}}$ is occasionally referred to as the effective mass number for a neutron scattered at the $i$ th level. The scattering probability is normally developed using a Legendre polynomial expansion to give:

$$
\sigma_{s}^{i}\left(E^{\prime} \rightarrow E\right)=\sigma_{s}^{i}\left(E^{\prime}\right) \frac{(A+1)^{2}}{2 E^{\prime} \tilde{A}\left(E^{\prime}\right)} \sum_{l=0}^{\infty} \frac{(2 l+1)}{2} p_{i}^{l}\left(E^{\prime}\right)^{i} P_{l}\left(\mu_{0}\right)
$$

The approach involving development of the probability according to Legendre polynomials as $\mu_{0}$ rather than $\mu=\cos \theta$ is based on the fact that the collision is considered isotropic at the center of mass frame (but not in the laboratory frame). We shall see in the chapter on the Boltzmann equation how transition from one to the other may be effectively managed.

### 2.2 Transmutations

(Mayo 1998, p62)
Neutrons, which are uncharged particles, interact very little with the electron cloud and do not have to overcome the electrostatic repulsive forces due to positively charged protons in the nucleus. They can reach the nucleus at very low speeds, and even lower than those of thermal agitation in the nucleus itself.

$$
{ }_{0}^{1} n+{ }_{92}^{235} U \rightarrow{ }_{92}^{236} U+\gamma \quad \text { radiative capture: }{ }_{92}^{235} U(n, \gamma){ }_{92}^{236} U
$$

Other particles may also reach the nucleus if they have sufficient energy:

$$
{ }_{2}^{4} \mathrm{He}+{ }_{7}^{14} \mathrm{~N} \rightarrow{ }_{1}^{1} \mathrm{H}+{ }_{8}^{17} \mathrm{O} \quad \alpha \quad \text { capture: }{ }_{7}^{14} \mathrm{~N}(\alpha, p){ }_{8}^{17} \mathrm{O}
$$

The capture process involves absorption of the incident particle which creates an excited composite nucleus, allowing re-emission of the ejected particle (Fig. 2.6):

When the energy of the incident particle is below 50 MeV , the compound nucleus constitutes the principal mechanism of nuclear reactions. Since the Louis de Broglie wavelength is far greater than the characteristic size of nucleons, the incident particle reacts with the entire nucleus and not just with its nucleons. The capture of a neutron or another particle may statistically result in several different products. We speak of exit channels, corresponding to entry channels, which may also be multiple (Cameron 1982, p20) (Fig. 2.7).

Thus, the excited ${ }_{13}^{27} A l^{*}$ nucleus may be formed by numerous entry channels and will result in exit channels that may also be multiple:

$$
\left.\begin{array}{l}
{ }_{0}^{1} n+{ }_{13}^{26} \mathrm{Al} \\
{ }_{2}^{4} \mathrm{He}+{ }_{11}^{23} \mathrm{Na} \\
\gamma+{ }_{13}^{27} \mathrm{Al} \\
\ldots
\end{array}\right\} \Rightarrow \begin{aligned}
& { }_{13}^{27} \mathrm{Al}^{*} \Rightarrow\left\{\begin{array}{l}
{ }_{13}^{26} \mathrm{Al}+{ }_{0}^{1} n \\
{ }_{11}^{23} \mathrm{Na}+{ }_{2}^{4} \mathrm{He} \\
{ }_{13}^{27} \mathrm{Al}+\gamma \\
\cdots
\end{array} .\right.
\end{aligned}
$$

When the nucleus resulting from the capture is different from the initial nucleus, we talk of transmutation, a term dear to mediaeval alchemists. During transmutation, the elements of the final state (after collision) are thus different from those of


Fig. 2.6 Capture showing an intermediate state: the compound nucleus


Infographie Margue $\dagger$


${ }_{13}^{27} A l^{*}$

${ }_{13}^{26} \mathrm{Al}$

A particle hits a target (here, a sodium 23 isotope).

A transient excited aluminum 27 isotope is created. This is the intermediate nucleus.

The excited isotope emits a neutron and forms a ${ }_{13}^{26} \mathrm{Al}$ nucleus.

Fig. 2.7 Reaction ${ }_{11}^{23} \mathrm{Na}(\alpha, n){ }_{13}^{26} \mathrm{Al}$
the initial state (before collision). Transmutation was first identified by Rutherford in 1919 and proven by photography undertaken in 1925 by Patrick Blackett ${ }^{4}$ :

$$
{ }_{2}^{4} \mathrm{He}+{ }_{7}^{14} N \rightarrow{ }_{1}^{1} H+{ }_{8}^{17} \mathrm{O}
$$

As with fission, the intermediate nucleus theory assumes that the target nucleus absorbs the particle before fragmenting according to several possible decay channels.

### 2.2.1 Absorption

Absorption indicates that the incident particle is absorbed by the target. Absorption of a neutron is written as follows:

[^33]$$
{ }_{0}^{1} n+{ }_{Z}^{A} X \rightarrow{ }_{Z}^{A+1 *} X
$$

The ${ }^{A+1}{ }_{Z}^{*} X$ nucleus is generally excited at around $6-7 \mathrm{MeV}$ above the ground state. Strictly speaking, absorption consists of transmutation since it follows the definition of a change in quantum state of the target, while use of the term transmutation is restricted to reactions involving changes in the chemical bodies between the initial and final states. In the case of absorption, the same chemical body is found in the final state, but in the form of another isotope.

### 2.2.2 (n, $\gamma$ ) Neutron Capture or Radiative Capture

This type of absorption is written as:

$$
{ }_{0}^{1} n+{ }_{Z}^{A} X \rightarrow{ }_{Z}^{A+1 *} X \rightarrow{ }_{Z}^{A+1} X+h v
$$

or more schematically:

$$
\begin{equation*}
\text { Neutron capture: }{ }_{0}^{1} n+{ }_{Z}^{A} X \rightarrow{ }_{Z}^{A+} X+E_{\gamma} \tag{2.4}
\end{equation*}
$$


(The Marguet collection)

An important example in the physics of uranium reactors is the fertile capture of the isotope ${ }_{92}^{238} \mathrm{U}$ to form fissile ${ }_{94}^{239} \mathrm{Pu}$ (Cameron 1982, p68):

$$
\left\{\begin{array}{l}
{ }_{0}^{1} n+{ }_{92}^{238} U \rightarrow{ }_{92}^{239} U+\gamma \\
{ }_{92}^{239} U \rightarrow{ }_{93}^{239} N p+{ }_{-1}^{0} e^{-} \text {by } \beta^{-} \\
{ }_{93}^{239} N p \rightarrow{ }_{94}^{239} \mathrm{Pu}+{ }_{-1}^{0} e^{-} \text {by } \beta^{-}
\end{array}\right.
$$

The capture of ${ }_{94}^{239} P u$ is, however, sterile in a $P W R$ since it results in a non-fissile isotope, ${ }_{94}^{240} \mathrm{Pu}$ (although in a fast neutron reactor, ${ }_{94}^{240} \mathrm{Pu}$ is fissile):

$$
{ }_{0}^{1} n+{ }_{94}^{239} P u \rightarrow{ }_{94}^{240} P u
$$

### 2.2.3 (n, $\alpha$ ) Capture

This type of neutron capture produces an $\alpha$ particle. An important capture of this type for the physics of $P W R \mathrm{~s}$ is the high-probability capture of ${ }_{5}^{10} B$, according to the reaction:

$$
{ }_{0}^{1} n+{ }_{5}^{10} B \rightarrow\left\{\begin{array}{cl}
{ }_{5}^{7} L i+{ }_{2}^{4} \mathrm{He}+2.793 \mathrm{MeV} & \text { in } 6 \% \text { of cases } \\
{ }_{3}^{7} L i^{*}+{ }_{2}^{4} \mathrm{He}+2.313 \mathrm{MeV} \quad \text { in } 94 \% \text { of cases }
\end{array}\right.
$$

The first excitation level of ${ }_{3}^{7} L^{3} i$ is 0.480 MeV and energy $Q$ of the reaction is 2.793 MeV , which accounts for the energy of 2.313 MeV of the second reaction. ${ }_{5}^{10} B$ is a potent neutron absorbing material that is introduced into the water in $P W R$ in the form of boric acid in order to control the nuclear reaction rate. It should be noted that the inverse reaction, i.e. $(\alpha, n)$ capture on light nuclei present in $P W R s$ such as oxygen 17 , oxygen 18 , nitrogen 14 and lithium 7 , can occur and produces a weak but detectable inherent source ${ }^{5}$, which increases in $M O X$ fuels due to the activity of plutonium 238.

### 2.2.4 Other Forms of Capture

Numerous other forms of capture exist, such as $(n, 2 n)$ captures, which are threshold reactions that become possible at an energy corresponding to $(A+1) / A$ times the binding energy of the last additional neutron of the target. The coefficient $(A+1) / A$

[^34]allows recoil energy in the nucleus to ensure conservation of movement (Price et al. 1957, p141):
$$
{ }_{0}^{1} n+{ }_{92}^{238} U \rightarrow{ }_{0}^{1} n+{ }_{0}^{1} n+{ }_{92}^{237} U
$$

Other more exotic forms of capture also exist, such as $(n, 3 n),(n, \alpha n),(n, p)$, and ( $n, p n$ ) captures, etc. At the energies involved in water reactors, only $(n, 2 n)$ and $(n, \alpha)$ captures are likely. Higher energy is required for the emergence of greater numbers of emitted particles.

### 2.2.5 High-Energy Reactions

At high energies (between 10 and 100 MeV ), the nucleus may be considered by incident neutrons as an opaque medium. By analogy with optics, the diffraction of neutrons is similar to the diffraction of light through an opaque object having the same shape and size as the nucleus. The nucleus may be considered as a translucent medium having the following absorption cross-section:

$$
\Sigma=\rho \sigma
$$

where $\rho$ is the mean density of the nucleus and $\sigma=\left[Z \sigma_{n p}+(A-Z) \sigma_{n n}\right] / A$ is the mean neutron/nucleus scattering cross-section, where $\sigma_{n p}$ and $\sigma_{n n}$ are respectively the cross-sections characterizing the probability of neutron/proton and neutron/ neutron interaction. We shall examine this notion of cross-sections in more detail below. This relatively simple approach provides an adequate explanation of interactions involving high-energy neutrons.

### 2.2.6 Energy Balance

(Mayo 1998, p83)
Nuclear reactions are subject to the fundamental laws of the conservation of total energy, momentum and charge. Let us use the following generic reaction in which $x$ is a light incident particle, $X$ is the target, and $y$ and $Y$ are the products of the reaction:

$$
x+X \rightarrow Y+y
$$

with: $E_{x}, E_{X}, E_{Y}, E_{y}$ the kinetic energies (if $X$ is the target, $E_{X}=0$ )

$$
m_{x}, M_{X}, M_{Y}, m_{y} \text { the masses at rest. }
$$

The energy balance (conservation of total energy) is written as follows:

$$
\left(m_{x}+M_{X}\right) c^{2}+E_{x}+E_{X}=\left(M_{Y}+m_{y}\right) c^{2}+E_{Y}+E_{y}
$$

The total energy of the reaction is given by:

$$
Q=\left(m_{x}+M_{X}\right) \cdot c^{2}-\left(M_{Y}+m_{y}\right) c^{2}=E_{Y}+E_{y}-E_{X}-E_{x}
$$

If $Q>0$, the reaction is exothermic (or exo-energetic). If $Q<0$, the reaction is endothermic. In the latter case, it may only occur through the kinetic energy, $e_{x}$, provided by the incident particle, and the reaction is said to be a threshold reaction. If one of the resulting particles is a photon, we replace its kinetic energy and the rest mass energy by $h \nu$. For all nuclear reactions except scattering, the balance of the rest mass is not conserved. The kinetic energy balance before and after collision is modified by term $Q$ in relation to that established for collisions with elastic scattering. We shall use the same notations (i.e. $\otimes$ in the center of mass framework, after collision) as in the calculation already described for elastic scattering, with a reaction energy term specific to a threshold reaction (Fig. 2.8):
$\left\{\begin{array}{ll}\forall i \in\{x, X\} & E_{i \otimes}=\frac{1}{2} m_{i} v_{i \otimes}{ }^{2}=\frac{1}{2} m_{i}\left|\overrightarrow{v_{i}}-\overrightarrow{V_{G}}\right|^{2} \quad \text { with } \\ \forall j \in\{y, Y\} & E_{j \otimes}=\frac{1}{2} m_{j} v_{j \otimes}{ }^{2}=\frac{1}{2} m_{j}\left|\overrightarrow{V_{j}}=\frac{m_{x} \overrightarrow{v_{x}}+m_{X} \overrightarrow{V_{X}}}{m_{x}+m_{X}}\right|^{2}\end{array}\right.$ with $\quad \overrightarrow{V_{G}^{\prime}}=\frac{m_{y} \overrightarrow{v_{y}}+m_{Y} \overrightarrow{V_{Y}}}{m_{y}+m_{Y}}$
since: $\overrightarrow{v_{x}}-\overrightarrow{V_{G}}=\overrightarrow{v_{x}}-\frac{m_{x} \overrightarrow{v_{x}}+m_{X} \overrightarrow{V_{X}}}{m_{x}+m_{X}}=\frac{m_{X}}{m_{x}+m_{X}}\left(\overrightarrow{v_{x}}-\overrightarrow{V_{X}}\right)$
and: $\overrightarrow{V_{X}}-\overrightarrow{V_{G}}=\overrightarrow{V_{X}}-\frac{m_{x} \overrightarrow{v_{x}}+m_{X} \overrightarrow{V_{X}}}{m_{x}+m_{X}}=\frac{m_{x}}{m_{x}+m_{X}}\left(\overrightarrow{V_{X}}-\overrightarrow{v_{x}}\right)$
giving: $E_{x \otimes}=\frac{1}{2} \frac{m_{x} m_{X}^{2}}{\left(m_{x}+m_{X}\right)^{2}}\left|\overrightarrow{v_{x}}-\overrightarrow{V_{X}}\right|^{2}=\frac{1}{2} \frac{m_{x} m_{X}^{2}}{\left(m_{x}+m_{X}\right)^{2}}\left(v_{x}^{2}+V_{X}^{2}-2 \overrightarrow{v_{x}} \cdot \overrightarrow{V_{X}}\right)$
and $E_{X \otimes}=\frac{1}{2} \frac{m_{X} m_{x}^{2}}{\left(m_{x}+m_{X}\right)^{2}}\left|\overrightarrow{V_{X}}-\overrightarrow{v_{x}}\right|^{2}=\frac{1}{2} \frac{m_{X} m_{x}^{2}}{\left(m_{x}+m_{X}\right)^{2}}\left(v_{x}^{2}+V_{X}^{2}-2 \overrightarrow{v_{x}} \cdot \overrightarrow{V_{X}}\right)$
and summed: $E_{x \otimes}+E_{X \otimes}=E_{x}+E_{X}-\underbrace{\frac{1}{2} \frac{m_{x} m_{X}}{m_{x}+m_{X}}\left|\frac{m_{x} \overrightarrow{v_{x}}+m_{X} \overrightarrow{V_{X}}}{m_{x}+m_{X}}\right|^{2}}_{E_{G}}$


Fig. 2.8 Non-elastic scattering in center-of-mass framework

$$
\text { in identical fashion: } E_{y \otimes}+E_{Y \otimes}=E_{y}+E_{Y}-\underbrace{\frac{1}{2} \frac{m_{y} m_{Y}}{m_{y}+m_{Y}}\left|\frac{m_{y} \overrightarrow{v_{y}}+m_{Y} \overrightarrow{V_{Y}}}{m_{y}+m_{Y}}\right|^{2}}_{E_{G}^{\prime}}
$$

The reaction energy is given by:

$$
Q=E_{Y}+E_{y}-E_{X}-E_{x}=E_{Y \otimes}+E_{y \otimes}-E_{X \otimes}-E_{x \otimes}+E_{G}^{\prime}-E_{G}
$$

Since $\quad M_{Y} \overrightarrow{V_{Y \otimes}}+m_{y}{\overrightarrow{v_{y}}}_{\otimes}=\overrightarrow{0}$, we have $\quad M_{Y} E_{Y \otimes}=m_{y} E_{y \otimes}$.
Similarly, $M_{X} \overrightarrow{V_{X}}+m_{x} \overrightarrow{v_{x}}=\overrightarrow{0}$, giving $M_{X} E_{X \otimes}=m_{x} E_{x \otimes}$. Finally, we have:

$$
\begin{equation*}
\text { Energy balance: } Q=\left(\frac{m_{y}}{M_{Y}}+1\right) E_{y \otimes}-\left(\frac{m_{x}}{M_{X}}+1\right) E_{x \otimes}+E_{G}^{\prime}-E_{G} \tag{2.5}
\end{equation*}
$$

The special case in which the target is fixed in the laboratory framework $\left(\overrightarrow{V_{X}}=\overrightarrow{0}\right)$ enables the results to be simplified:

$$
\left\{\begin{array}{l}
E_{x \otimes}=\left(\frac{M_{X}}{M_{X}+m_{x}}\right)^{2} E_{x} \quad E_{X \otimes}=\frac{m_{x} M_{X}}{\left(M_{X}+m_{x}\right)^{2}} E_{x} \quad E_{G}=\frac{m_{x}}{M_{X}+m_{x}} E_{x} \\
E_{y \otimes}=\frac{M_{Y}}{M_{Y}+m_{y}}\left[Q+\left(1-\frac{m_{x}}{M_{Y}+m_{y}}\right) E_{x}\right] \quad E_{Y \otimes}=\frac{m_{y}}{M_{Y}+m_{y}}\left[Q+\left(1-\frac{m_{x}}{M_{Y}+m_{y}}\right) E_{x}\right]
\end{array}\right.
$$

Thus, for any reaction that occurs, the energy equation $Q=E_{Y}+E_{y}-E_{X}-E_{x}$ shows that if the target and particles after collision are assumed (in theory) to be immobile, it is necessary that $E_{x}>-Q$ at least in order for the reaction to be possible. However, although necessary, this condition is not sufficient to ensure conservation of the momentum. The formulae of $E_{y \otimes}$ and $E_{Y \otimes}$ show the following to be necessary:

$$
Q \geq-\left(1-\frac{m_{x}}{M_{Y}+m_{y}}\right) E_{x} \quad \text { i.e. } \quad E_{x} \geq-\frac{Q}{\left(1-\frac{m_{x}}{M_{Y}+m_{y}}\right)}>-Q
$$

The corrective term $m_{x} /\left(M_{Y}+m_{y}\right)$ may be negligible if the mass of the incident particle is small in relation to that of the target, but for a small target correction must be considered.

### 2.3 Fission

(Physics Chemistry Fission 1969; Endt and Smith 1962, p42; Lilley 2001, p263)
Fission of an atom of uranium 235 struck by a slow (thermal) neutron generally produces two fission fragments, and less commonly three (in the case of ternary fission, one of the products is normally extremely light ${ }^{6}$ ), known as fission products. Fission also produces some fission neutrons, and a great deal of energy compared to the mass used:

$$
{ }_{0}^{1} n+{ }_{92}^{235} U \rightarrow{ }_{56}^{137} B a+{ }_{36}^{96} K r+3{ }_{0}^{1} n+E_{\gamma}
$$

This reaction is only one example among others since another neutron may cause fission of a heavy nucleus according to a different mode of fission, and the balance will produce other fission products, such as the following for example:

$$
{ }_{0}^{1} n+{ }_{92}^{235} U \rightarrow{ }_{54}^{135} \mathrm{Xe}+{ }_{38}^{99} \mathrm{Sr}+2{ }_{0}^{1} n+E_{\gamma}
$$

Under experimental circumstances, it may be seen that fission can generally produce two or three neutrons, and less commonly more neutrons (up to 6) or fewer neutrons (a single emitted neutron). The mean number of neutrons depends on the fissioning nucleus (this number increases with heavy nuclei) and the energy of the incident neutron (the umber increases with increasing energy). The mean number of neutrons emitted is of the order of 2.5 for ${ }_{92}^{235} U$. Fission, a key reaction in nuclear fission reactors, will be examined in more detail later.

### 2.4 Fusion

(Dolan 1982; Jancel and Kahan 1963; Landshoff 1957, 1958; Mayo 1998, p241; Pai 1962; Stacey 1981; Survey of Phenomena in Ionized Gases 1968)

[^35]The fusion of two light atoms also releases a great quantity of energy. It results in the emission of neutrons having a kinetic energy superior to that of fission, of the order of 14 MeV , and generally produces a heavier particle.

$$
\begin{gathered}
\underbrace{{ }_{1}^{2} H}_{\text {Deuterium }}+\underbrace{{ }_{1}^{3} H}_{\text {Tritium }} \rightarrow{ }_{2}^{4} \mathrm{He}+{ }_{0}^{1} n+17.59 \mathrm{MeV} \\
{ }_{1}^{2} H+{ }_{1}^{2} H \rightarrow\left\{\begin{array}{l}
{ }_{2}^{3} H e+{ }_{0}^{1} n(+3.27 \mathrm{MeV}) \\
{ }_{1}^{3} H+{ }_{1 p}^{1}(+4.00 \mathrm{MeV})
\end{array}\right.
\end{gathered}
$$

In relation to the atomic mass involved, fusion releases far more energy than fission. Moreover, it employs isotopes that are abundant on earth (for instance isotopes present in water), in contrast with uranium, and it generates few highly radioactive fission products (in fact, radioactive fusion products have a short halflife), and it is thus highly attractive from an industrial standpoint, independently of the technical problems that must be overcome. For fusion reactions to take place, the Coulomb barrier must be overcome, which requires either an extremely high speed of the incident particle, or a very high temperature of the target to harness Brownian motion, and, generally, a very large magnetic field in order to contain the totally ionized gas (plasma) in a sufficiently small volume, in order to control the fusion process. All of these conditions have been combined in a Tokamak fusion reactor (Smirnov 2001).

### 2.5 Cross Sections

### 2.5.1 Basic Definitions

(Mayo 1998, p115)
The probability of interaction between particle and matter brings up the notion of cross sections. This probability of interaction with matter over a distance $d x$ is defined by the dimensionless value $\Sigma d x$. It is logically proportional to the path length, and since it is dimensionless, $\Sigma$ represents the dimension of the inverse of length (Fig. 2.9).

This value is called the macroscopic cross section and it is a property of the material being crossed. By geometric analogy, this probability is also proportional to the number of nuclei $N$ per $\mathrm{cm}^{3}$ :

$$
d P(x)=\Sigma d x=N \sigma d x
$$

with $\sigma$ thus defined as a microscopic cross section $\left[\mathrm{cm}^{2}\right]$.
Since $\Sigma d x$ is the probability of interaction with matter, $1-\Sigma d x$ is logically the probability of no interaction occurring over the distance $d x$. Where $Q(x)$ is the probability of a neutron travelling from the origin to $x$ without interaction, we can

Fig. 2.9 Interaction of a neutron with matter


Fig. 2.10 Ratio of probability of interaction to concentration of target nuclei

calculate the probability of a neutron reaching $x+d x$ from the probability of it reaching $x$, i.e. $Q(x)$, and of it not interacting throughout the distance $d x$, which is by definition $(1-\Sigma d x)$ :

$$
Q(x+d x)=Q(x)(1-\Sigma d x)
$$

thus, by integration: $Q(x)=e^{-\Sigma x}$
Where $P(x)$ is the probability of an initial interaction between $x$ and $x+d x$ (and thus not an interaction on $0 x$ ) (Fig. 2.10):

$$
P(x) d x=e^{-\Sigma x} \Sigma d x
$$

The integral of this probability over an infinite path is: $\int_{0}^{\infty} e^{-\Sigma x} \Sigma d x=1$, meaning that the neutron will necessarily have an interaction, but also that $P(x)$ is a normalized probability in the mathematical sense of the term. The mean free path between the origin and the first collision (thus between two successive collisions) is given by:


Fig. 2.11 Exponential attenuation of a neutron beam $I(x)=I_{0} \cdot e^{-\Sigma_{t} x}$

$$
\lambda_{[\mathrm{cm}]} \equiv \frac{\int_{0}^{\infty} x P(x) d x}{\int_{0}^{\infty} P(x) d x}=\int_{0}^{\infty} e^{-\Sigma x} d x=\frac{1}{\Sigma}
$$

For a neutron travelling at speed $v$, the flight time between two collisions is $l=\lambda /$ $v=1 /(\Sigma v)$. At the end of the mean free path, the intensity of the beam of neutrons is weakened by a factor of $e$ (the Napier's constant). If a narrow beam of monokinetic neutrons with speed $v$ is now projected perpendicularly onto a target material, the neutron current is the name given to the intensity $I$ of neutrons per $\mathrm{cm}^{2}$ and per second. To simplify the problem, we will consider that any interaction between a neutron and the material will either result in the scattered neutron leaving the beam, or else disappearing purely and simply through absorption. The probability of complete interaction is named the total cross section $\Sigma_{t}$. The variation in intensity, $d I$, measured along the axis of the beam due to interaction between neutrons and matter, is given by (Fig. 2.11):

$$
d I=-I \Sigma_{t} d x
$$

The neutron current of speed $v$ is attenuated on passing through the foil. This method enables the total cross section to be determined, provided there are incident monokinetic neutrons.

### 2.5.2 Measurement of Cross Sections

(Harvey 1970)
An ingenious experimental setup can be used to select neutrons at a desired speed (monokinetic). The required neutrons may be filtered using an apparatus called chopper (Egelstaff 1965, p57) which works by means of a rotating cylindrical wheel containing overlaid strips of cadmium and aluminum (Fig. 2.12 and Photo 2.1), in the axis of a beam of multi-kinetic neutrons. These neutrons are produced by a source of short pulses, with the impulses being separated by a longer latency time. The layers of aluminum, a substance that is relatively transparent for neutrons, allows the passage of those neutrons whose speed enables them to be transmitted


Fig. 2.12 Chopper used to obtain monokinetic neutrons


Photo 2.1 Chopper: the layers of aluminum are clearly discernible. After (Progress in Nuclear Energy Vol 2 1958, pp160-161)
without being stopped by a layer of cadmium, which, in contrast, is totally opaque for thermal neutrons. By varying the speed of rotation of the selector, the distance between the pulse source and the detector, and the time lapse between emission of the pulse and discernible opening of the sensor, it is possible to filter neutrons travelling at a given speed (Kahan 1963, p67; Neutron time-of-flight 1961).

### 2.5.3 Notion of Flux and Reaction Rate

In reality, within the reactor, neutrons obviously do not all travel at the same speed and, above all, not in the same direction. We therefore define an order of scale, the neutron flux (in neutrons per $\mathrm{cm}^{2}$ and per second), which is the product of the concentration of neutrons and their speed:

$$
\begin{equation*}
\text { Neutron flux: } \Phi_{\left[\mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}\right]} \equiv n_{\left[\mathrm{n} / \mathrm{cm}^{3}\right]} v_{[\mathrm{cm} / \mathrm{s}]} \tag{2.6}
\end{equation*}
$$

The unit of flux suggests, by analogy, a flow rate of neutrons crossing a surface. However, in contrast with the current, where neutrons travel perpendicularly through a unit of area, flux here corresponds rather to a volume: all of the neutrons in one $\mathrm{cm}^{3}$ are counted and then multiplied by their respective speed. The term flux is thus somewhat misleading and in the past, numerous authors have sought to redefine an alternative term, although unsuccessfully, since the word flux is now too widely used in neutron physics to be abandoned. Since neutrons have different energies, and thus different speeds, i.e. $\vec{v}(E)$ in direction $\vec{\Omega}$, and numbers $n(E)$, it is possible to define angular flux in an element of solid angle $d \Omega$ and in an element with energy differential $d E$ such that:

$$
\begin{equation*}
\text { Angular flux: } \varphi(\vec{r}, \vec{\Omega}, E) d \Omega d E=n(\vec{r}, \vec{\Omega}, E) v(E) d \Omega d E \tag{2.7}
\end{equation*}
$$

The non-relativistic neutron speed is given by its kinetic energy, $v=\sqrt{2 E / m}$, hence the notion of flux spectrum (flux depends on energy). The integrated flux is defined by integration on the solid angle and the energy:

$$
\Phi(\vec{r})=\int_{4 \pi} d \Omega \int_{0}^{\infty} \varphi(\vec{r}, \vec{\Omega}, E) d E=n(\vec{r}) \bar{v}
$$

where $\bar{v} \equiv \frac{\int_{0}^{\infty} n(\vec{r}, E) v d E}{\int_{0}^{\infty} n(\vec{r}, E) d E}$ is the mean speed over the spectrum.
For each reaction, a specific cross section is defined: $\sigma_{(n, \gamma)}, \sigma_{(n, \alpha)}$, $\sigma_{\text {scattering }, \ldots}$. as well as logical reconstruction rules:

$$
\left\{\begin{aligned}
\sigma_{\text {total }} & \equiv \sigma_{\text {absorption }}+\sigma_{\text {scattering }} \\
\sigma_{\text {absorption }} & \equiv \sigma_{\text {capture }}+\sigma_{\text {fission }}
\end{aligned}\right.
$$

Since the order of magnitude of microscopic cross sections is very small, we use a subunit of the SI unit, the barn ${ }^{7}$, equivalent to $10^{-24} \mathrm{~cm}^{2}$. For a neutron of speed $v$, the probability of interaction during $d t$ is $\Sigma d x=\Sigma v d t$. Where $n$ is the density of incident neutrons (in neutrons per $\mathrm{cm}^{3}$ ), the number of interactions is given by $n \Sigma v d t$, that is per unit of time, i.e. $n \Sigma v$ interactions per second. The reaction rate is $R \equiv \Sigma \Phi$ in reactions $\cdot \mathrm{cm}^{-3} \cdot \mathrm{~s}^{-1}$.

[^36]
### 2.5.4 Resonance

The cross section of a given material (e.g. a metal) may be measured by placing an extremely thin foil of this material in a flux of monokinetic incident neutrons (travelling at the same speed) of known energy. We simply measure attenuation of the neutron beam and deduce the corresponding microscopic cross-section using the law of attenuation. Measurement of cross sections shows them to be dependent not only on the type of material involved, naturally, but also on the energy of the incident neutron. In general, the cross section decreases as the neutron speed increases (since matter is more "transparent" to faster neutrons). However, at low energies, sudden variations occur in the cross section as a function of energy, as if neutrons at a certain energy level are captured virtually systematically.

In classical Newtonian mechanics, the probability of interception of the neutron would be constant, if we disregard the Brownian movement of the target. These capture peaks are in fact due to quantum mechanics, in which the nucleus is modeled not as a large bead, but rather as a resonant cavity, with the neutron being seen as a wave (in similar fashion to an electron in the formalism of Louis de Broglie). When the "neutron" wave resonates with the target cavity at certain frequencies, there is every chance of the neutron being absorbed. The cross section (Fig. 2.13) is represented in terms of increasing energy.

This area of sudden variation is referred to as the "resonance region". Only those neutrons having a post-collision energy different to the energy of the residences will be able to escape the latter. Analyzing the levels of excitation of the compound nucleus ${ }^{A+}{ }_{Z}^{1} X$, we find the position of the resonances of a particular reaction. When a neutron interacts with a target nucleus ${ }_{Z}^{A} X$, in addition to the kinetic energy of the neutron, $E_{n}$, in the center of mass frame, the binding energy, $B_{n}(A+1, Z)$ is also released such that $B_{n}(A+1, Z)=\left[M(A, Z)+m_{n}-M(A+1, Z)\right] c^{2}$, and it is

Fig. 2.13 Cross sections with resonances

distributed in the compound nucleus, which it then excites. Taking as an example nitrogen ${ }_{7}^{15} N$, this nucleus may be formed by different reactions (on the left) and produce various disintegration pathways (on the right):

$$
\left.\begin{array}{l}
{ }_{7}^{14} N+{ }_{0}^{1} n \\
{ }_{6}^{14} C+{ }_{1}^{1} p \\
{ }_{5}^{11} B+{ }_{2}^{4} \mathrm{He} \\
\cdots
\end{array}\right\} \rightarrow{ }_{7}^{15} N^{*} \rightarrow\left\{\begin{array}{l}
{ }_{7}^{14} N+{ }_{0}^{1} n \\
{ }_{6}^{14} C+{ }_{1}^{1} p \\
{ }_{5}^{11} B+{ }_{2}^{4} \mathrm{He} \\
{ }_{7}^{15} N+\gamma_{0} \\
{ }_{7}^{15} N^{*}+\gamma_{1} \\
\cdots
\end{array}\right.
$$

If a neutron (taken as having no speed) is captured by ${ }_{7}^{14} N$, the resulting nucleus ${ }_{7}^{15} \mathrm{~N}$ recovers the binding energy of the new neutron in the form of excitation energy based on the principle that the mass of the compound nucleus is lower than the total mass of ${ }_{7}^{14} N$ and of the initial neutron. If the neutron possesses kinetic energy in its center of mass, this further increases the excitation energy. Several possibilities then arise: first, ${ }_{7}^{15} N^{*}$ may de-excite to its ground state, emitting a $\gamma_{0}$ photon. Nuclear de-excitation of the nucleus may also occur with emission of a $\gamma_{1}$ photon of even lower energy, leaving the ${ }_{7}^{15} N^{*}$ nucleus in an excited state. Another outcome is possible, namely elastic (or inelastic) scattering, which will produce ${ }_{7}^{14} \mathrm{~N}$ and a scattering neutron.

If we analyze for instance the ( $n, p$ ) and ( $n, \alpha$ ) capture cross sections of ${ }_{7}^{14} N$, we see resonances that coincide with the levels of excitation of ${ }_{7}^{15} N$ taking into account the shift of 10.75 MeV corresponding to the binding energy $B_{n}(A+1, Z)$ of this nucleus. The same conclusion applies to the $(p, n)$ cross-section of ${ }_{6}^{14} C$, this time with a shift of 10.15 MeV corresponding to the binding energy of a proton of ${ }_{7}^{15} N$. Because of the multiple levels, not described in our simplified schema (Fig. 2.14), coupled with Heisenberg's uncertainty principle, the resonances widen around the levels, or even overlap with one another, thus "softening" the peaks. We may even define negative resonances to describe the levels not reachable by the neutron and situated just below the 10.75 MeV for neutron capture threshold. However, the width of these theoretical resonances affects the shape of the low-energy cross section. By way of illustration, Fig. 2.15 shows the broad resonance for fission of ${ }_{92}^{235} U$ (JEF 2.2) at 0.3 eV and the start of narrow resonances as of 1 eV . Capture resonances are symmetrical when the scattering resonances are clearly asymmetrical. We will see later that this phenomenon is due to an interference effect with the potential scattering cross-section, and we will analyze this phenomenon in the chapter on the Doppler effect. Resonances may follow one another rapidly, as in the case of the $(n, \gamma)$ capture resonances of ${ }_{92}^{238} U$ (Fig. 2.16), which can still be described in the resolved region.

One way of weighing successive resonances in the discernible region is to compare the resonance integral of two isotopes, defined mathematically as follows:


Fig. 2.14 Levels of ${ }_{7}^{15} N^{7}$ after (Lederer and Shirley 1978): On the left is the complete and extremely complex scheme of the energy levels of the isotope ${ }_{7}^{15} N^{7}$, as found in databanks, with different possible transitions and spin. If the capture process results in the formation of a compound nucleus ${ }_{7}^{15} N^{7} *$ excited at level $E_{n}$, de-excitation can occur with emission of a $\gamma_{0}$ photon towards the ground state, but also, depending on the cross sections of the entry channels represented on the right of the schema, with the emission of neutron, proton or helium particles

$$
\begin{equation*}
\text { Resonance integral: } I_{[\mathrm{barn}]}=\int_{E=E_{t h}}^{E=+\infty} \sigma(E)_{[\mathrm{barr}]} d E / E \tag{2.8}
\end{equation*}
$$



Fig. 2.15 Cross section of ${ }_{92}^{235} U$ up to 5 eV (data from $J E F 2$ )

In practice, since the limits of the integral have no physical meaning, the epithermal resonance integral, found in libraries of cross-sections, is defined as follows:

$$
I_{[\mathrm{barn}]}=\int_{E=0.5 \mathrm{eV}}^{E=100 \mathrm{keV}} \sigma(E)_{[\mathrm{barn}]} d E / E
$$

Not all isotopes necessarily have resonances, and thus ${ }_{5}^{10} B$ presents a total crosssection almost perfectly of $1 / v$ (or $1 / \sqrt{E}$ ), as shown in Fig. 2.17. At low energy, $1 / v$ behavior, occasionally referred to as Gamov's law, is highly systematic for all isotopes of less than 0.1 eV (Fig. 2.15).

A noteworthy fact of particular use for simplified calculations is that the ( $n, \alpha$ ) cross-section of ${ }_{5}^{10} B$ is a law perfectly in $1 / v$ below 100 keV (Cameron 1982, p32). The extremely marked ( $n, \alpha$ ) capture by this isotope (cross-section at $2200 \mathrm{~m} / \mathrm{s}$ $\sigma_{0}=3840.5$ barns $_{[J E F 2]}$, epithermal resonance integral $I=1724.37$ barns $_{[J E F 2]}$ ), present in natural boron, is used particularly in light-water reactors to control chain reactions, but also in the protective materials industry (Photo 2.2). Natural boron containing between $18 \%$ and $20 \%$ (depending on its source) of ${ }_{5}^{10} B$ is placed in the reactor water by diluting boric acid. If we suppose a perfect $1 / v$ law, its


Fig. 2.16 Cross sections of ${ }_{92}^{238} U$ between 100 eV and 1000 eV (data from JEF2)


Fig. 2.17 Cross sections of ${ }_{5}^{10} B$ (data from JEF2)


Photo 2.2 French advertisement from 1957 for "made in France" protective materials containing boron (The Marguet collection)
resonance integral in barns may be readily calculated (between 0.5 eV and 100 keV depending on the definition of the resonance integral):

$$
\begin{gathered}
I_{[\text {barr] }]} \equiv \int_{E=0.5 \mathrm{eV}}^{E=100 \mathrm{keV}} \sigma(E)_{[\text {barn }]} \frac{d E}{E}=\int_{E=0.5 \mathrm{eV}}^{E=100 \mathrm{keV}} \frac{\sigma_{0} v_{0}}{\sqrt{\frac{2 E}{m}}} \frac{d E}{E}=\left[-\frac{2 \sigma_{0} v_{0}}{\sqrt{\frac{2 E}{m}}}\right]_{E=0.5 \mathrm{eV}}^{E=100 \mathrm{keV}}=\left[-2 \sigma_{0} \sqrt{\frac{E_{0}}{E}}\right]_{E=0.5 \mathrm{eV}}^{E=100 \mathrm{keV}} \\
I_{[\text {barn }]}=2 \sigma_{0}\left[\sqrt{\frac{0.0253}{0.5}-} \sqrt{\frac{0.0253}{100} 10^{3}}\right]=1723.93 \quad \text { barns } \approx I=1724.37_{[J E F 2]}
\end{gathered}
$$

Excellent coherence may be noted between the calculation of the resonance integral assuming a $1 / v$ law and the value given in the $J E F 2$ library. It should be noted that the unit of $I$ is the barn, which means that $\sigma(E)$ is also expressed in barns ${ }^{8}$. Certain rare isotopes present resonances below 0.5 eV , notably in the important

[^37]

Fig. 2.18 Cross sections of ${ }_{54}^{135} \mathrm{Xe}$ (data from JEF2)
case of ${ }_{54}^{135} \mathrm{Xe}$, which is the most absorbent fission product in the thermal spectrum, and which weighs considerably in the neutron balance (over $2000 \mathrm{pcm}^{9}$ in a $P W R$ ) (Fig. 2.18).

Generally speaking, scattering cross sections are constant over a wide energy range. For example, the scattering cross-section of ${ }_{1}^{1} \mathrm{H}$ (Fig. 2.19), the main moderator isotope in water reactors, exhibits an extremely stable plateau of around 20 barns between 0.1 eV and 10 keV . Note the classic $1 / v$ form at very low energy due to Doppler broadening at $20^{\circ} \mathrm{C}$. This concept will be described later in a specific chapter.

The case of scattering in crystal, the general theory of which is developed in (Progress in Nuclear Physics Vol 1 1960a, p185), contains an interesting particularity. Above around 1 eV , scattering is chiefly due to the potential cross-section, i.e. scattering by the field potential of the nucleus (Egelstaff and Poole 1969, p6). If the wavelength of the incident neutron is far greater than the radius of the target nucleus, the potential cross-section is virtually energy-independent. Below 0.01 eV , different scattering processes occur, and these are clearly dependent on temperature according to a $1 / v$ curve.

At around 0.005 eV , when neutrons undergo coherent scattering by adjacent atoms as in a crystal or a molecule, interference is noted between the scattered neutron waves to the extent that the Louis de Broglie wavelength of the neutron is around $10^{-8} \mathrm{~cm}$, i.e. the order of magnitude of the inter-atomic space in a network.

[^38]

Fig. 2.19 Scattering cross-section of ${ }_{1}^{1} H$ (data from $J E F 2$ )


Fig. 2.20 Bragg cut-off for the scattering cross-section of crystalline beryllium after [P.K Job, M. Srinivasan: Exploitation of Bragg cut-off phenomenon for improved albedo in Berylliumreflected minimum critical mass systems, Nuclear Science and Engineering, 85, 422 (1983)]

This phenomenon, which is well known with regard to x-rays, is known as Bragg scattering and results in the appearance of a threshold (Fig. 2.20) in the curve of the cross section (Bragg cut-off) that is given by the following formula (Glasstone and Sesonske 1994, p94), (Bekurts and Wirtz 1964, p17):

$$
E_{\text {Bragg }[\mathrm{eV}]}=\frac{2.04 \times 10^{-4}}{d_{[n m]}^{2}}
$$

where $d$ is the maximum distance between two rows of atoms in the crystal. This phenomenon has little effect inside a reactor since at 300 K , only $5 \%$ of neutrons with Maxwellian distribution are below 0.005 eV . However, it enables non-intrusive investigation of matter, and gave rise to neutron optics (Diffraction et diffusion des neutrons (Diffraction and diffusion of neutrons) 1964).

Within a reactor, materials composed of several isotopes are found. If we ignore the effects of binding of molecules, the microscopic cross sections combine by simple addition (Meghreblian and Holmes 1960, p47; Mayo 1998, p135):

$$
\Sigma_{H_{2} O}=\Sigma_{H}+\Sigma_{O}=N_{H} \sigma_{H}+N_{O} \sigma_{O}
$$

The fact that a water molecule contains two hydrogen atoms per oxygen atom is reflected in the fact that $N_{H}=2 N_{O}$. This is applied by composing the abundances of natural chemical bodies, for example:

$$
N_{\text {Boron }} \sigma_{\text {Boron }}^{a}=N_{{ }_{5} B} \sigma_{5_{5} B}^{a}+N_{{ }_{5} B} \sigma_{11}^{a} B
$$

At low energy, the effects of molecular binding, particularly in the case of light water and heavy water, significantly increase the scattering cross-section (Bennet 1981, p39), cancelling out the law of composition of macroscopic cross sections (Fig. 2.21):

Cross sections show great variation (e.g. for ${ }_{92}^{235} U$, Fig. 2.22) as a function of energy, and for this reason precise calculation of the neutron spectrum of a reactor

Fig. 2.21 Effect of binding of water molecule on the scattering cross-section: the cross-section of free atoms is constant while the crosssection of the water molecule increases practically linearly at low energies



Fig. 2.22 Cross sections of ${ }_{92}^{235} U$ (data from JEF2)
requires the cross sections to be arranged by energy group. The mean cross-section for the energy group $\left[E_{1}, E_{2}\right]$ is defined as follows:

Mean macroscopic cross section by energy group:

$$
\begin{equation*}
\bar{\Sigma} \equiv \frac{\int_{E_{1}}^{E_{2}} \Sigma(E) \Phi(E) d E}{\int_{E_{1}}^{E_{2}} \Phi(E) d E}=\frac{\int_{E_{1}}^{E_{2}} \Sigma(E) n(E) v d E}{\int_{E_{1}}^{E_{2}} \Phi(E) d E} \tag{2.9}
\end{equation*}
$$

We speak of flux in the group $\left[E_{1}, E_{2}\right]$ or integrated fux: $\Phi=\int_{E_{1}}^{E_{2}} \Phi(E) d E$.
Generalization to a single group is performed by setting $E_{1}=0$ and $E_{2}=+\infty$. Calculations for $P W R$ are frequently performed in two energy groups with a cut-off at 0.625 eV which corresponds to the cut-off in the absorbing isotope of cadmium: ${ }_{48}^{113} \mathrm{Cd}$.

This isotope pf cadmium presents a giant capture resonance at 0.172 eV , the wings of which extend to 0.6 eV , and we may thus consider that any neutrons under 0.625 eV would be absorbed by a piece of cadmium foil. We can therefore measure the ratio of thermal flux to total flux by placing a counter in the area to be measured, successively surrounded with and without a cadmium foil (Fig. 2.23).

Natural cadmium is a strong neutron absorber, primarily because of its isotope ${ }_{48}^{113} \mathrm{Cd}$ ( $12.22 \%$ in natural cadmium). This resonance makes cadmium practically "impermeable" (we refer to a black body) to neutrons below 0.3 eV . Since its


Fig. 2.23 Cross sections of ${ }_{48}^{113} \mathrm{Cd}$ (data from JEF2)
resonance integral ( $I=394.072$ barns $)$ is lower than that of ${ }_{5}^{10} B$, it is in fact fairly ineffective at energies greater than 10 eV compared with ${ }_{5}^{10} B$. However, in the thermal region, it is an excellent neutron absorber, like xenon. At two energy groups, the energy condensations are written as follows:

$$
\left\{\begin{array}{lrl}
\text { Fast } & \Phi_{1}=\int_{E_{\text {cuuoff }}}^{+\infty} \Phi(E) d E & \Sigma_{1}=\frac{\int_{E_{C}}^{+\infty} \Sigma(E) \Phi(E) d E}{\Phi_{1}} \\
\text { Thermal } & \Phi_{2}=\int_{0}^{E_{\text {cuuoff }}} \Phi(E) d E & \Sigma_{2}=\frac{\int_{0}^{E_{C}} \Sigma(E) \Phi(E) d E}{\Phi_{2}}
\end{array}\right.
$$

The total reaction rate is obtained by summing the rates for the two groups: $\Sigma_{1} \Phi_{1}+\Sigma_{2} \Phi_{2}$. The reaction rates are cumulative in the same way as the integrated fluxes $\Phi_{\text {total }}=\Phi_{1}+\Phi_{2}$. In choosing the type of cross-section, we choose the type of reaction rate:

$$
R_{\text {absorption }}=\Sigma_{a} \Phi, \quad R_{\text {fission }}=\Sigma_{f} \Phi, \quad R_{\text {production }}=\nu \Sigma_{f} \Phi
$$

It is in fact possible to define an energy production rate $\kappa \Sigma_{f} \Phi$ in which $\kappa$ is the energy liberated by fission. The energy production rate is thus an expression of power by volume in $\left[\mathrm{J} / \mathrm{cm}^{3} / \mathrm{s}\right]$ or in $\left[\mathrm{W} / \mathrm{cm}^{3}\right]$. Where $\kappa$ is given in MeV (of the order


Fig. 2.24 Classification of nuclear reactions by target, after (Soodak 1955)
of 200 MeV ), the energy rate is expressed in $\left[\mathrm{MeV} / \mathrm{cm}^{3} / \mathrm{s}\right]$. Figure 2.24 provides a summary of the interaction of neutrons with the various isotopes. Below a mass number of 25 , i.e. for light nuclei, the main reaction is scattering, with the notable exception of ( $n, \alpha$ ) reactions on ${ }_{5}^{10} B$ and ${ }_{3}^{6} L i$, as well as the ( $n, p$ ) reaction on ${ }_{2}^{3} \mathrm{He}$. Only radiative capture ( $n, \gamma$ ) is able to excite the target nucleus, with its clearly isolated resonances. The first excited level is generally above a few MeV. For nuclei of intermediate mass (between 25 and 80), and for low energies ( $\leq 1 \mathrm{keV}$ ) and moderate energies ( $\leq 500 \mathrm{keV}$ ), the predominant reactions are elastic scattering and radiative capture, with clearly separated resonances. Inelastic scattering is generally impossible since the first excited level is situated several hundred keV above the ground state of the compound nucleus. ( $n, p$ ) and ( $n, \alpha$ ) reactions are weak due to the strong Coulomb barrier. Regarding low-energy heavy nuclei, only neutrons having a moment $l=0$ are able to interact and produce fissions, radiative captures or inelastic scattering. The very high Coulomb barrier prevents the emission of charged particles. The width of the absorption resonances is far greater than that of the neutron involved in scattering. This idea will be discussed in more depth in the chapter on resonant absorption. Even $Z$, odd $A$ nuclei have large fission cross sections while even $Z$, even $A$ nuclei mainly tend towards capture. For intermediate energies, the neutron resonance width of heavy isotopes increases as $\sqrt{E}$ while the absorption width remains relatively constant. Inelastic reactions and the emission of charged particles are highly unlikely. At high energies ( $\geq 500 \mathrm{keV}$ ), both intermediate and heavy nuclei present non-negligible inelastic scattering cross-sections, as well as the emission of charged particles, while the space between levels diminishes and the capture cross-section increases with mass number (although it decreases
with energy). The neutron resonance width decreases. Even $Z$, even $A$ nuclei become fissile.

### 2.6 Nuclear Fission

In October 1934, after positing the theory of $\beta$ radioactivity, Enrico Fermi (1901-1954) understood the phenomenon of the slowing down of neutrons as they passed through light substances, and he noted that the probability of interaction with matter increased inversely with speed ( $1 / v$ ). He was awarded the Nobel Prize in 1938 for his work on $\beta$ decay. This provided him with the opportunity to "go west", in other words to leave Fascist Italy, where he feared government excesses (his wife was of Jewish origin). In 1936-1937, interested in artificial radioactivity, Fermi built his own "neutron canons" by mixing beryllium powder and radon (a naturally gaseous element, radium was far too expensive at the time for the limited means of the University of Rome). Radon is an $\alpha$ emitter and its interaction with beryllium produces neutrons in accordance with the reaction already interpreted by Chadwick:

$$
{ }_{2}^{4} \mathrm{He}+{ }_{4}^{9} \mathrm{Be} \rightarrow{ }_{6}^{12} \mathrm{C}+{ }_{0}^{1} n
$$

Fermi used his canon to bombard all species of chemicals bought from a local shop by fellow physicist Emilio Segrè, another future Nobel Prize winner (who according to Fermi's wife was sent out with an errand list and shopping bag!) starting with the lightest substances. He obtained no radioactivity with hydrogen, boron, carbon or nitrogen, but just as he was about to give up, he noted strong radioactivity in fluorine, and also in other heavier chemical substances. Bombarding uranium in the same way, he noted intense radioactivity produced by several radioactive elements but he was unable to recognize any particular period of radioactivity. He claimed to have discovered element 93 ("An Italian produces the element 93 by bombarding uranium!" ran the New York Times headline) but others thought that it was in fact only protactinium $(Z=91)$ or another element close to uranium but lighter.

In any event, these studies were of great interest to German radiochemist Otto Hahn (1879-1968) and Austrian chemist Lise Meitner (1878-1968). Hahn had worked as a young man with Rutherford in Montreal. Together with Lise Meitner, he replicated Fermi's experiments at the Kaiser-Wilhelm Institute in Berlin. Alongside chemist Fritz Strassman (1902-1980), he carried out in-depth studies on the uranium capture reaction products, but in July 1938, Lise Meitner, who was of Jewish origin, was forced to flee Nazi Germany. Hahn and Strassman continued their experiments in 1939 and, while seeking traces of radium using a chemical

Photo 2.3 In the early 1960s, Karl Wirtz shows Otto Hahn (right) the plans of Germany's first research reactor, FR2 (1961-1981), in Karlsruhe (photo Karlsruhe)

priming technique involving barium, they noted that they were unable to isolate radium purely and simply because it was barium ${ }^{10}$. Using an ingenious method to scan air, they also detected the radioactive gases krypton and xenon (Nahmias 1953, p96) (Photo 2.3).

Lise Meitner interpreted the experiment in Stockholm ${ }^{11}$, ascribing it to the fission of uranium! This was a stunning discovery for a time when the atom was still considered indivisible (Photo 2.4).

In Paris, Frédéric Joliot immediately provided photographic evidence of the trajectory of a fission fragment in a Wilson chamber, and together with Von Halban and Kowarski ${ }^{12}$, he showed that fission produced $2-3$ neutrons of a mean energy of 2 MeV (Mathieu 1991, p235). Fission of an atom of uranium 235 almost always produces two fission fragments, known as fission products, as well as neutrons known as prompt fission neutrons since they are produced practically

[^39]

Photo 2.4 Otto Hahn's work table on which we see the device used to detect fission. This fairly simple equipment enabled production of sufficient fissions for chemical detection of the presence of barium (photo Karlsruhe)
instantaneously. The excess mass that disappears is transformed into energy. Ternary fission (which produces three fragments, one of which is generally extremely light) is very rare ( $<1$ case per 100,000 fissions), and is generally ignored, except of course where the focus is on production of a light isotope such as tritium for example. Normally, binary fissions of the following type occur:

$$
{ }_{0}^{1} n+{ }_{92}^{235} U \rightarrow{ }_{56}^{137} B a+{ }_{36}^{96} K r+3{ }_{0}^{1} n+E_{\gamma}
$$

It should be noted that fission of the uranium atom can produce a large number of statistically different fission products. The intermediate nucleus theory assumes absorption of the incident neutron, resulting in a highly unstable nucleus that breaks up like a drop of water (Born 1971, p298) (Fig. 2.25).

In 1939, N. Bohr and J.A. Wheeler, taking up the ideas postulated by Gamov in 1929, proposed the liquid drop model (Valentin 1982a, b, p130), in which the nucleus is represented as a group of nucleons whose equilibrium is governed by antagonistic forces: a cohesive force associated with the surface tension of the nuclear "liquid' that maintains cohesion, and a dislocation force due to Coulomb repulsion between protons (Pollard and Davidson 1956, p230). When the system undergoes a collision during interaction with an external particle, it vibrates around its position of spherical equilibrium. If the oscillation is too great and allows a particular geometrical configuration to be reached, that results in sufficient narrowing at the center (the saddle point) and corresponding to the maximum

${ }_{92}^{236} U^{*}$

${ }_{92}^{236} U^{*}$


A slow incident neutron strikes an atom of uranium 235.

The resulting compound nucleus is highly unstable. It oscillates around its spherical equilibrium position.

The nucleus is deformed and reaches thesaddle point before breaking (the liquid drop model) into two fragments of virtually identical size. In rare cases, a third, extremely light fission product appears...
... together with anumberof neutrons (two or three, according to the individual case) and intense energy liberation (around 200 MeV per fission). The majority of this energy is dissipated in the form of kinetic energy of the recoil fragments. Given the size of these fragments (fission products), this energy is rapidly transferred to the medium and the fragments are practically stopped dead in their tracks.

Fig. 2.25 Liquid drop model of fission
potential energy of the system, the nucleus breaks into two smaller drops. The saddle point is reached in trans-uranium elements by adding energy of around 6 MeV , but in some cases this potential barrier may be overcome via tunneling effect, which accounts for the spontaneous fissions noted with certain actinides. The chances of fission are increased with slow neutrons while a fast neutron at 14 MeV (the maximum energy of a neutron generated by fission) has a very low probability of causing a fission itself.

### 2.6.1 Fission Energy

Fission energy may be calculated using the Aston curve for binding energy by calculating loss of mass. For a fission producing ${ }_{56}^{137} \mathrm{Ba}$ and ${ }_{36}^{96} \mathrm{Kr}$, the energy liberated by the fission is of the order of:
$\underbrace{8.6 \mathrm{MeV} / \text { nucleon } \times 96}_{825.6}+\underbrace{8.5 \mathrm{MeV} / \text { nucleon } \times 137}_{1164.5}-\underbrace{7.6 \mathrm{MeV} / \text { nucleon } \times 236}_{1793.6}=196.5 \mathrm{MeV}$
i.e. near the level of 200 MeV calculated by W. Heisenberg in 1930. If each fission produces several neutrons, it may be seen that under sufficiently propitious circumstances, certain neutrons will be able to recreate a fission. Frédéric Joliot, Hans Von Halban and Lew Kowarski were the first to consider that the $\nu$ neutrons created by fission might be used to fission another atom of ${ }_{92}^{235} U$. This phenomenon is known as a chain reaction. The fission energy of ${ }_{92}^{235} U$ may be broken down as follows:

$$
\begin{aligned}
E_{\text {kinetic (recoil) }} \text { of fission products } & =166.2 \pm 1.3 \mathrm{MeV} \\
E_{\gamma \text { prompt }} & =8.0 \pm 0.8 \mathrm{MeV} \\
E_{\gamma \text { delayed }} & =7.2 \pm 1.1 \mathrm{MeV} \quad E_{\text {neutrinos }}=9.6 \pm 0.5 \mathrm{MeV} \text { lost } \\
E_{\beta} & =7.0 \pm 0.3 \mathrm{MeV} \\
E_{\text {kinetic }} \text { of neutrons } & =4.8 \pm 0.1 \mathrm{MeV} \\
\text { Total recoverable } & =193.2 \mathrm{MeV}
\end{aligned}
$$

The energy of the neutrinos is lost, since there is practically no interaction between matter and these particles, so they escape from the reactor. The kinetic energy $E_{\text {kinetic }}$ (in MeV ) of the fission products increases overall as the mass of the fissioning nucleus grows (Table 2.3). By way of illustration:
(Baur 1985, p180) provides a precise breakdown of the fission energy for the main fissile isotopes. Prompt $\gamma$ rays are emitted within $10^{-9} \mathrm{~s}$ after fission. The total energy of these $\gamma$ rays is around 8 MeV , and 10 or so photons are emitted per fission (7.4 photons for ${ }_{92}^{235} U+n$ ). The remaining $\nu-1$ neutrons that were not involved in fission are generally captured by nuclei in the reactor structure $(n, \gamma)$ (except from those escaping from the reactor), and they give back a mean 6 MeV , i.e. $6(\nu-1) \approx$ 8.5 MeV to the total, since $\nu \approx 2.4$ (Table 2.4).

The probability of fission for fissile isotopes is dependent on the energy of the incident neutron and is characterized by the cross section. Several heavy isotopes have high fission cross-sections, particularly the isotopes ${ }_{92}^{233} U$, ${ }_{92}^{235} \mathrm{U},{ }_{94}^{239} \mathrm{Pu},{ }_{94}^{241} \mathrm{Pu}$ and ${ }_{95}^{242 m} \mathrm{Am}$. Others are only fissile at high energy levels, and these are generally isotopes having an even mass number and an even atomic number: ${ }_{90}^{232} \mathrm{Th}, \quad{ }_{92}^{238} \mathrm{U}, \quad{ }_{94}^{240} \mathrm{Pu}$ and ${ }_{94}^{242} \mathrm{Pu}$. The isotope ${ }_{92}^{235} \mathrm{U}$ is extremely fissile with thermal neutrons while ${ }_{92}^{238} U$ is fissile only with the fastest neutrons in the spectrum (above 1 MeV ). Since a single inelastic scattering event is generally

Table 2.3 Kinetic energy (in MeV) of fission products for several fissile systems ( $+n=$ neutroninduced fission, $s p=$ spontaneous fission)

| ${ }_{90}^{229} \mathrm{Th}+n$ | ${ }_{92}^{233} U+n$ | ${ }_{92}^{235} U+n$ | ${ }_{94}^{239} \mathrm{Pu}+n$ | ${ }_{94}^{241} \mathrm{Pu}+n$ |
| :--- | :--- | :--- | :--- | :--- |
| 160 | 163 | 166 | 172 | 174 |
| ${ }_{94}^{242} \mathrm{Pu} \mathrm{sp}$ | ${ }_{96}^{242} \mathrm{Cm} \mathrm{sp}$ | ${ }_{96}^{244} \mathrm{Cm} \mathrm{sp}$ | ${ }_{98}^{252} \mathrm{Cf} s p$ | ${ }^{254} \mathrm{Fm} \mathrm{sp}$ |
| 174 | 197 | 185 | 185 | 176 |

Table 2.4 Total fission energy including capture effects

| Fissioning nucleus | ${ }_{92}^{235} \mathrm{U}$ | ${ }_{92}^{238} \mathrm{U}$ | ${ }_{94}^{239} \mathrm{Pu}$ | ${ }_{94}^{241} \mathrm{Pu}$ |
| :--- | :--- | :--- | :--- | :--- |
| Recovered energy (MeV/fission), including $E(n, \gamma)$ | 201.7 | 205.0 | 210.0 | 212.4 |

Table 2.5 Numbers of neutrons emitted by fission (after (Uhrig 1970, p52))

| $\nu$ | $p(\nu)$ | $\nu p(\nu)$ | $\nu^{2} p(\nu)$ |
| :--- | :--- | :--- | :--- |
| 0 | 0.03 | 0 | 0 |
| 1 | 0.16 | 0.16 | 0.16 |
| 2 | 0.33 | 0.66 | 1.32 |
| 3 | 0.30 | 0.90 | 2.70 |
| 4 | 0.15 | 0.60 | 2.40 |
| 5 | 0.03 | 0.15 | 0.75 |
| 6 | $<0.001$ | $\approx 0$ | $\approx 0$ |
| total | 1 | $\bar{\nu}=2.47$ | $\overline{\nu^{2}}=7.33$ |

sufficient to ensure transition of a neutron to above 100 keV , and thus to below the 1 MeV threshold, it is legitimate to consider that ${ }_{92}^{238} \mathrm{U}$ is only fissile with fission neutrons from the initial collision. It should also be noted that the rapid fission crosssection of ${ }_{92}^{235} U$ is of the same order of magnitude as that of ${ }_{92}^{238} U$, which is why enrichment of around $5 \%$ with ${ }_{92}^{235} U$ is sufficient to maintain a chain reaction in the rapid spectrum in a reactor considered as infinite. For a fast reactor of reasonable size, the minimum enrichment required to maintain such a reaction may be taken as $10 \%$ in ${ }_{92}^{235} U$.

In a water-moderated reactor, natural uranium is not sufficient to attain critical mass due to parasite captures by the water, and the fuel must therefore be enriched in ${ }_{92}^{235} U$. Enrichment of around $3 \%$ enables an industrially acceptable critical size to be attained. In $3.7 \%$ UOX PWR fuel, the following mean numbers of neutrons emitted per fission may be used:

$$
\bar{\nu}_{235}{ }_{99} U=2.47 \quad \bar{\nu}_{232} U=2.78
$$

These mean values summarize the distribution of fission neutrons. For example, for ${ }_{92}^{235} U$, the number of neutrons produced per fission ranges from 0 to 6 (Table 2.5).

### 2.6.2 Spontaneous Fission

Although we are chiefly concerned with neutron-induced fission, it is useful to know about the phenomenon of spontaneous fission that occurs with certain heavy nuclei. Spontaneous fission consists of segmentation into two fission products that is not induced by shock. This rare form of fission is characterized by a branching ratio on the decay constant and it obeys the same rules as disintegration. A heavy nucleus will therefore emit $\alpha$ radiation and undergo spontaneous fission with very slight branching. Thus, ${ }_{92}^{235} U$ has spontaneous fission branching of $3.76 \times 10^{-7} \%$, with the complement of 1 corresponding to the principal $\alpha$ decay. In general, the heavier the nucleus the greater the degree of spontaneous fission. Spontaneous fission occurs with nuclei having an even mass number (with the notable exception of ${ }_{92}^{235} \mathrm{U}$ and ${ }_{94}^{239} \mathrm{Pu}$ ).

### 2.6.3 Neutrons Produced by Fission

(Goldstein 1959, p46; Rockwell 1956, p32)
The mean number of neutrons, $\bar{\nu}$, emitted by fission depends on the fissile heavy nucleus in question and on the incident neutron energy. Experimental measurements show that there are two types of neutrons: prompt neutrons, which are produced practically instantaneously after fission of the nucleus (within less than $10^{-10}$ seconds following fission) and make up over $99 \%$ of neutrons; and delayed neutrons, which occur in small quantities and may be emitted a significant time after fission. Although they occur only in very small quantities, we shall see that delayed neutrons are crucial in achieving kinetic control of the reactor. The heavier the fissioning nucleus, the more neutrons it will produce on average. Similarly, the greater the energy of the incident neutron, the greater the number of neutrons produced (always as a mean value). The change in $\bar{\nu}$, which includes prompt and delayed neutrons, is practically linear, in accordance with the energy.

$$
\bar{\nu}(E)=\bar{\nu}_{\text {thermal }}+\frac{d \bar{\nu}}{d E} E
$$

By way of example, Howerton ${ }^{13}$ measured the following for ${ }_{96}^{242} \mathrm{Cm}$ : $\bar{\nu}(E)=3.44+0.172 E_{[\mathrm{MeV}]}$.

The values of $\bar{\nu}_{\text {thermal }}$ and $d \bar{\nu} / d E$ for different fissile systems are given in Table 2.6. Where $\chi(E)$ is the number of prompt neutrons emitted at energy $E$ and normalized to production of 1 neutron, normalization is as follows:

Table 2.6 Constants of mean neutrons emitted per induced fission (Evaluation and Testing of Actinide Cross Section, EPRI NP-1067, 1979 and Reactor Physics Constants—ANL-5800)

| $\bar{\nu}(E)=\bar{\nu}_{\text {thermal }}+\frac{d \bar{\nu}}{d E} E$ | $\bar{\nu}_{\text {thermal }}$ | $\frac{d \bar{\nu}}{d E}$ |
| :---: | :---: | :---: |
| ${ }^{2392} \mathrm{Th}$ | 2.047 | 0.1530 |
| ${ }_{92}^{233} U$ | 2.500 | 0.1150 |
| ${ }_{92}^{235} U$ | 2.430 | 0.1346 |
| ${ }_{92}^{238} U$ | 2.409 | 0.1385 |
| ${ }_{92}^{239} \mathrm{Pu}$ | 2.868 | 0.1106 |
| ${ }_{96}^{242} \mathrm{Cm}$ | 3.440 | 0.1720 |
| ${ }_{96}^{245} \mathrm{Cm}$ | 3.830 | 0.1900 |
| ${ }_{97}^{249}$ Bk | 3.410 | 0.2140 |

[^40]$$
\int_{0}^{\infty} \chi(E) d E=1
$$

The mean energy of the neutrons emitted is of the order of 2 MeV , and only $5 \%$ of emitted neutrons have an energy level above 5 MeV . In the 1950s, and in the absence of any sufficiently precise theory of fission, many empirical formulae were introduced in order to provide an analytical description of the fission spectrum. The following is an example of the Maxwellian type (Woods 1964):

$$
\chi(E) \equiv 2 a \sqrt{\frac{a E}{\pi}} e^{-a E}
$$

where for ${ }_{92}^{235} U$, the constant $a$ is around $0.775 \mathrm{MeV}^{-1}$. Whatever the value of the constant $a$, this empirical formula complies with normalization of the spectrum:

$$
\int_{0}^{\infty} \chi(E) d E=\int_{0}^{\infty} 2 a \sqrt{\frac{a E}{\pi}} e^{-a E} d E=\frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}\right)=1
$$

The mean neutron energy is given by:

$$
\int_{0}^{\infty} \chi(E) E d E=\int_{0}^{\infty} 2 a \sqrt{\frac{a E}{\pi}} E e^{-a E} d E=\frac{2}{a \sqrt{\pi}} \Gamma\left(\frac{5}{2}\right)=\frac{3}{2 a}
$$

i.e. 1.93 MeV for ${ }_{92}^{235} U$. Other identical Maxwellian approaches exist for the majority of fissile isotopes such as the formula for the number of neutrons emitted as a function of energy ${ }^{14}$, in which $T$ is called the Maxwell spectrum temperature (in MeV ):

$$
n(E)=C \sqrt{E} e^{-\frac{E}{T}}
$$

Normalization of this formula is such that:

$$
\int_{0}^{\infty} n(E) d E=\int_{0}^{\infty} C \sqrt{E} e^{-E / T} d E=C T^{\frac{3}{2}} \Gamma\left(\frac{3}{2}\right)=C \frac{\sqrt{\pi}}{2} T^{\frac{3}{2}}=\bar{\nu}
$$

The mean energy of the spectrum is given by the formula:

$$
\bar{E}=\frac{\int_{0}^{\infty} n(E) E d E}{\int_{0}^{\infty} n(E) d E}=\frac{C \frac{\sqrt{\pi}}{2} \frac{3}{2} T^{\frac{5}{2}}}{C \frac{\sqrt{\pi}}{2} T^{\frac{3}{2}}}=\frac{3 T}{2}
$$

[^41]Table 2.7 Maxwell coefficients describing the fission neutron spectrum $n(E)=C \sqrt{E} e^{-\frac{E}{T}}$

| Fissile nucleus | $T_{[\mathrm{MeV}]}$ | $C_{[-]}=2 \nu \pi^{-\frac{1}{2}} T^{-\frac{3}{2}}$ | $\bar{E}_{[\mathrm{MeV}]}=\frac{3 T}{2}$ | $\int_{0}^{\infty} n(E) d E=\nu$ |
| :--- | :--- | :--- | :--- | :--- |
| ${ }_{92}^{235} U+n$ | 1.290 | 1.872 | 1.935 | 2.430 |
| ${ }_{92}^{233} U+n$ | 1.306 | 1.888 | 1.959 | 2.497 |
| ${ }_{92}^{239} P u+n$ | 1.333 | 2.121 | 1.999 | 2.893 |
| ${ }_{98}^{252} \mathrm{Cf} s p$ | 1.420 | 2.504 | 2.130 | 3.756 |

according to this formulation: $\chi(E)=\frac{2}{\sqrt{\pi} T^{3}} \sqrt{E} e^{-E / T}=\frac{2}{T} \sqrt{\frac{E}{T \pi}} e^{-E / T}$
We find the previous formula in which $T$ assumes the role of $I / a$ (Table 2.7).
These values are provided for purely thermal incident neutrons. In an actual neutron spectrum, induction of fission is not limited to thermal neutrons. A Maxwell spectrum may be extrapolated taking the following as the mean energy ${ }^{15}$ :

$$
\bar{E}=0.78+0.621 \sqrt{1+\bar{\nu}}
$$

where $\bar{\nu}$ is the mean number of neutrons emitted by fission in the real spectrum. The spectrum:

$$
\chi(E)=\frac{2}{\sqrt{\pi} T^{\frac{3}{2}}} \sqrt{E} e^{-E / T}
$$

may be analytically integrated by parts if we wish to determine the proportion of neutrons in a given energy group $\left[E_{i}, E_{f}\right]$, without specific numeric integration since there exists a library of pre-tabulated functions, using the following error function:

$$
\operatorname{erf}(x)=\frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^{2}} d t=\frac{2}{\sqrt{\pi}} \int_{0}^{x^{2}} \frac{1}{2 \sqrt{t}} e^{-t} d t
$$

Indeed:

[^42]

Fig. 2.26 Fission spectrum for ${ }_{92}^{235} U: \quad \chi(E)=0.453 e^{-1.036 E} \operatorname{sh} \sqrt{2.29 E}$

$$
\begin{aligned}
\int_{E_{i}}^{E_{f}} \chi(E) d E & =\frac{2}{\sqrt{\pi}} \int_{E_{i}}^{E_{f}} \frac{1}{T^{\frac{3}{2}}} \sqrt{E} e^{-\frac{E}{T}} d E=\frac{2}{\sqrt{\pi}} \int_{\frac{E_{i}}{T}}^{\frac{E_{f}}{T}} \sqrt{t} e^{-t} d t \\
& =\frac{2}{\sqrt{\pi}}\left(-\left[\sqrt{t} e^{-t}\right]_{\frac{E_{i}}{T}}^{\frac{E_{f}}{T}}+\int_{\frac{E_{i}}{T}}^{\frac{E_{f}}{T}} \frac{1}{2 \sqrt{t}} e^{-t} d t\right)
\end{aligned}
$$

and thus:

$$
\int_{E_{i}}^{E_{f}} \chi(E) d E=\frac{2}{\sqrt{\pi}}\left(\sqrt{\frac{E_{i}}{T}} e^{-\frac{E_{i}}{T}}-\sqrt{\frac{E_{f}}{T}} e^{-\frac{E_{f}}{T}}\right)+\operatorname{erf}\left(\sqrt{\frac{E_{f}}{T}}\right)-\operatorname{erf}\left(\sqrt{\frac{E_{i}}{T}}\right)
$$

In the 1950 s , B. E. Watt proposed an empirical formulation ${ }^{16}$ valid between 0.1 MeV and 18 MeV that was widely used in the following form (Price et al. 1957, p146):

$$
\begin{equation*}
\text { Watt spectrum: } \chi(E)=C e^{-a E} \sinh \sqrt{b E} \tag{2.10}
\end{equation*}
$$

where $a=1 \mathrm{MeV}^{-1}, b=2 \mathrm{MeV}^{-1}$ and $C=0.48387$ for the isotope ${ }_{92}^{235} U$.
Since then, the term Watt spectrum has been commonly used to designate the fission spectrum, despite the fact that the exact formula proposed by Watt is not used in reality. Newer more precise coefficients have been provided by Lamarsh circa (1966): $a=1.036 \mathrm{MeV}^{-1}, b=2.29 \mathrm{MeV}^{-1}$ and $C=0.453$ for the isotope ${ }_{92}^{235} U$ (Fig. 2.26). The mean neutron energy is given by:

[^43]Table 2.8 Coefficients of the Watt fission neutron spectrum $\chi(E)=C e^{-a E} \operatorname{sh} \sqrt{b E}$

|  | Incident neutron energy | $a\left[\mathrm{MeV}^{-1}\right]$ | $b\left[\mathrm{MeV}^{-1}\right]$ |
| :--- | :--- | :--- | :--- |
| ${ }_{90}^{232} \mathrm{Th}+n$ | Thermal | 0.9184 | 1.6871 |
|  | 1 MeV | 0.9012 | 1.6316 |
|  | 14 MeV | 0.8547 | 1.4610 |
| ${ }_{92}^{233} \mathrm{U}+n$ | Thermal | 1.0235 | 2.5460 |
|  | 1 MeV | 1.0235 | 2.5460 |
|  | 14 MeV | 0.9964 | 2.6377 |
| ${ }_{92}^{235} \mathrm{U}+n$ | Thermal | 1.0121 | 2.2490 |
|  | 1 MeV | 1.0121 | 2.2490 |
|  | 14 MeV | 0.9728 | 2.0840 |
| ${ }_{92}^{238} \mathrm{U}+n$ | Thermal | 1.3449 | 3.4005 |
|  | 1 MeV | 1.1172 | 3.2953 |
|  | 14 MeV | 1.0359 | 2.8330 |
| ${ }_{92}^{239} \mathrm{Pu}+n$ | Thermal | 1.0352 | 2.8420 |
|  | 1 MeV | 1.0352 | 2.8420 |
|  | 14 MeV | 0.9479 | 2.3830 |
| ${ }_{92}^{240} \mathrm{Pu}$ | Spontaneous fission | 1.2516 | 4.9030 |
| ${ }_{92}^{242} \mathrm{Pu}$ | Spontaneous fission | 1.1995 | 4.4317 |
| 242 |  |  |  |
| 94 | Spontaneous fission | 1.1236 | 3.8480 |
| ${ }_{94}^{244} \mathrm{Cm}$ | Spontaneous fission | 1.1037 | 2.9260 |
| ${ }_{98}^{252} \mathrm{Cf}$ | Spontaneous fission | 0.9756 |  |

$$
E_{\text {mean }}=\frac{\int \chi(E) E d E}{\int \chi(E) d E}=1.98 \mathrm{MeV}
$$

Watt coefficients exist for the majority of fissile systems. Above, we present the values of the coefficients for the most widely used fissile systems (Table 2.8) and for three incident neutron energies: thermal energy, fission neutrons at 1 MeV , and fusion neutrons at 14 MeV .

### 2.6.3.1 Theoretical Fission Spectrum

The hyperbolic sine function proposed by Watt is derived from a calculation based on the hypothetical energy distribution of fission fragments. Let us suppose that neutrons are emitted in an isotropic fashion by fission products during slowing down in matter. The composition of the particle speeds is written as follows:

$$
v^{2}=v_{r}^{2}+V^{2}+2 V v_{r} \cos \psi
$$

where $v$ is the speed of the neutron (mass $m$ ) in the center of the laboratory, $V$ is the speed of the emitting fission product (mass $M$ ) in the center of the laboratory, and $v_{r}$ is the relative speed of the neutron in relation to its emitter. Since the mass of the
neutron is generally far lower than that of its emitter, we may consider that the center of mass of the emitter/neutron system is located in the fission product.


Velocity triangle
If $E=m v^{2} / 2$ is the kinetic energy of the neutron in the center of the laboratory and whose distribution we are seeking to establish, $\varepsilon=m v_{r}^{2} / 2$ is its "relative" kinetic energy, and $E_{F P}=M V^{2} / 2$ is the kinetic energy of the fission product, the composition of velocities indicates that the "relative' energy can range from $\varepsilon_{\min }=m\left(v^{2}-V^{2}\right) / 2$ for an emission angle of $\psi=0$ to $\varepsilon_{\max }=m\left(v^{2}+V^{2}\right) / 2$ for an angle of $\psi=\pi$.

If we assume neutron emission to be isotropic in the center of mass, this means that the probability of emission at a given angle is proportional to the solid angle:

$$
p(\Omega) d \Omega=\frac{d \Omega}{4 \pi}=\frac{2 \pi \sin \psi d \psi}{4 \pi}=\frac{\sin \psi d \psi}{2}
$$

Differentiating the velocity composition law taking $v_{r}$ as the constant, we find that (without accounting for the sign):

$$
2 v d v=2 V v_{r} \sin \psi d \psi
$$

Thus:

$$
\frac{\sin \psi d \psi}{2}=\frac{v}{2 V v_{r}} d v=\frac{\sqrt{\frac{2 E}{m}}}{2 V \sqrt{\frac{2 \varepsilon}{m}}} \sqrt{\frac{2}{m}} \frac{1}{2 \sqrt{E}} d E=\frac{1}{2 V \sqrt{2 m \varepsilon}} d E
$$

If we now assume that the distribution of neutrons by "relative' energy is Maxwellian and of the form:

$$
m(\varepsilon) d \varepsilon=\frac{2}{T \sqrt{\pi T}} \sqrt{\varepsilon} e^{-\frac{\varepsilon}{T}} d \varepsilon
$$

of which the integral over the entire energy range is:

$$
\int_{0}^{+\infty} m(\varepsilon) d \varepsilon=\frac{2}{\sqrt{\pi}} \int_{0}^{+\infty} \sqrt{\frac{\varepsilon}{T}} e^{-\frac{\varepsilon}{T}} \frac{d \varepsilon}{T}=\frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}\right)=1
$$

The energy T is the "temperature" of the Maxwell spectrum. The energy distribution of neutrons is then given by:

$$
\chi(E) d E=\int_{\varepsilon=\varepsilon_{\min }}^{\varepsilon=\varepsilon_{\max }} m(\varepsilon) d \varepsilon \frac{1}{2 V \sqrt{2 m \varepsilon}} d E=\frac{1}{V \sqrt{2 \pi m T}} \int_{\varepsilon=\varepsilon_{\min }}^{\varepsilon=\varepsilon_{\max }} e^{-\frac{\varepsilon}{T}} \frac{d \varepsilon}{T} d E
$$

After integration between the limits $\varepsilon_{\min }=\left(\sqrt{E}-\sqrt{\frac{m}{M} E_{P F}}\right)^{2}$ and $\varepsilon_{\max }=$ $\left(\sqrt{E}+\sqrt{\frac{m}{M} E_{P F}}\right)^{2}$, we obtain a hyperbolic sine function:

$$
\chi(E) d E=\frac{2}{V \sqrt{2 \pi m T}} e^{-\frac{m E_{P F}}{M T}} e^{-\frac{E}{T}} \operatorname{sh}\left(\frac{2 \sqrt{\frac{m E_{P F} E}{M}}}{T}\right) d E
$$

By selecting the numerical values $T \approx 1 \mathrm{MeV}$ and $m E_{F P} / M \approx 0.5 \mathrm{MeV}$ it is possible to formulate a first approximation of the experimental distribution. Under these hypotheses:

$$
\chi(E) d E=\frac{2}{V \sqrt{m} \sqrt{2 \pi e}} e^{-E} \operatorname{sh}(\sqrt{2 E}) d E
$$

It may also be seen that:

$$
\frac{m E_{F P}}{M}=\frac{m \frac{1}{2} M V^{2}}{M}=\frac{m V^{2}}{2}=0.5 \mathrm{MeV} \text { thus } V \sqrt{m}=1 \mathrm{MeV}^{0.5}
$$

Taking $a=\sqrt{\frac{2}{\pi e}} \approx 0.484$, we finally obtain a "Watt" type formula for $E$ expressed in MeV :

$$
\chi(E) d E=a e^{-E} \operatorname{sh}(\sqrt{2 E}) d E
$$

Note that the expression $m E_{F P} / M=0.5 \mathrm{MeV}$ implies uniform behavior among fission products. It would have been more accurate to consider a Maxwellian distribution of the energy of fission products having a mean of $166 / 2=83 \mathrm{MeV}$, since 166 MeV is the total recoil kinetic energy of the two fission products, as well as a curve for the distribution of mass of the fission products. However, this
hypothesis would greatly complicate the calculation without significant improvement in precision.

### 2.6.3.2 Average Energy of Fission Neutrons

The mean value of the previous spectrum may be calculated analytically:

$$
\bar{E} \equiv \int_{E=0}^{E=+\infty} E \chi(E) d E=a \int_{E=0}^{E=+\infty} E e^{-E} \operatorname{sh}(\sqrt{2 E}) d E=a \int_{E=0}^{E=+\infty} E e^{-E} \frac{e^{+\sqrt{2 E}}-e^{-\sqrt{2 E}}}{2} d E
$$

Using a change in variable $\sqrt{E}=x \pm \frac{1}{\sqrt{2}} \quad$ or $\frac{1}{2 \sqrt{E}} d E=d x$, we obtain:

$$
\begin{gathered}
\frac{\bar{E}}{a} \equiv \int_{x=-\frac{1}{\sqrt{2}}}^{x=+\infty}\left(x+\frac{1}{\sqrt{2}}\right)^{3} e^{-\left(x+\frac{1}{\sqrt{2}}\right)^{2}} e^{+\sqrt{2}\left(x+\frac{1}{\sqrt{2}}\right)} d x \\
-\int_{x=+\frac{1}{\sqrt{2}}}^{x=+\infty}\left(x-\frac{1}{\sqrt{2}}\right)^{3} e^{-\left(x-\frac{1}{\sqrt{2}}\right)^{2}} e^{-\sqrt{2}\left(x-\frac{1}{\sqrt{2}}\right)} d x \\
\frac{\bar{E}}{a} \equiv \sqrt{e}\left(\int_{x=-\frac{1}{\sqrt{2}}}^{x=+\infty}\left(x+\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x-\int_{x=+\frac{1}{\sqrt{2}}}^{x=+\infty}\left(x-\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x\right)
\end{gathered}
$$

These integrals may be judiciously segmented to obtain:

$$
\begin{gathered}
\frac{\bar{E}}{a \sqrt{e}} \equiv \int_{x=-\frac{1}{\sqrt{2}}}^{x=0}\left(x+\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x+\int_{x=0}^{x=+\infty}\left(x+\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x \\
-\int_{x=0}^{x=+\infty}\left(x-\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x+\int_{x=0}^{x=+\frac{1}{\sqrt{2}}}\left(x-\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x
\end{gathered}
$$

Noting that:

$$
\int_{x=0}^{x=+\frac{1}{\sqrt{2}}}\left(x-\frac{1}{\sqrt{2}}\right)^{3} e^{-x^{2}} d x=-\int_{y=-\frac{1}{\sqrt{2}}}^{y=0}\left(y+\frac{1}{\sqrt{2}}\right)^{3} e^{-y^{2}} d y
$$

Using the factorial for real numbers: $\Gamma(n) \equiv \int_{x=0}^{x=+\infty} x^{n-1} e^{-x} d x$ we obtain:

$$
\begin{aligned}
& \int_{x=0}^{x=+\infty} x^{2} e^{-x^{2}} d x=\int_{y=0}^{y=+\infty} \frac{\sqrt{y}}{2} e^{-y} d y \\
& =\frac{1}{2} \Gamma\left(\frac{3}{2}\right)=\frac{\sqrt{\pi}}{4} \text { and } \int_{x=0}^{x=+\infty} e^{-x^{2}} d x=\int_{y=0}^{y=+\infty} \frac{1}{2 \sqrt{y}} e^{-y} d y=\frac{1}{2} \Gamma\left(\frac{1}{2}\right)=\frac{\sqrt{\pi}}{2}: \\
& \frac{\bar{E}}{a \sqrt{e}}=\int_{x=0}^{x=+\infty} \frac{6 x^{2}+1}{\sqrt{2}} e^{-x^{2}} d x=\frac{1}{\sqrt{2}} \frac{6 \Gamma\left(\frac{3}{2}\right)+\Gamma\left(\frac{1}{2}\right)}{2}=\frac{1}{2 \sqrt{2}} \frac{8 \sqrt{\pi}}{2}=\sqrt{2 \pi} \\
& \text { With } \quad a=\sqrt{\frac{2}{\pi e}}, \quad \text { we obtain: } \quad \bar{E}=2 \mathrm{MeV}
\end{aligned}
$$

The reader may adapt this result in accordance with the specific parameters $a$ and $b$ for the isotope under consideration.

### 2.6.4 Prompt Fission Photons

(Goldstein 1959, p58; Rockwell 1956, p34)
The fission diagram in the liquid drop model seen earlier contains $7 \gamma$ rays that are produced instantaneously. This figure tallies with reality since the exact figure for the fissile nucleus ${ }_{92}^{235} U$ is 7.028 per fission (this is obviously a mean number: in most cases, $7 \gamma$ rays are emitted, and more rarely, 8 ). The spectrum of prompt $\gamma$ rays, i.e. the number $n\left(E_{\gamma}\right)$ of $\gamma$ rays at a corresponding $\gamma$ energy level, is illustrated


Fig. 2.27 Prompt $\gamma$ spectrum for ${ }_{92}^{235} U$


Fig. 2.28 Prompt $\gamma$ energy spectrum for ${ }_{92}^{235} U$
below for fission of ${ }_{92}^{235} U$. It may be correctly approximated ( $n\left(E_{\gamma}\right)=8.0 e^{-1.1 E_{\gamma}}$ ) by $n\left(E_{\gamma}\right)=8.0 e^{-1.1 E_{\gamma}}$ with $E_{\gamma}$ in MeV . Note that since fission products also produce photons according to the approximate law $n_{F P}\left(E_{\gamma}\right)=6.0 e^{-1.1 E_{\gamma}}$, the sum of the two contributions gives the total number of photons produced by a fission. The energy of these prompt $\gamma$ rays, $m\left(E_{\gamma}\right)=E_{\gamma} n\left(E_{\gamma}\right)$, is also plotted. The sum of these energies, (i.e. the total energy of $\gamma$ rays denoted $E_{\gamma \text { prompt }}$ in the energy balance seen in the breakdown of the energy liberated by fission of ${ }_{92}^{235} U$ ) is 7.8265 MeV (Figs. 2.27 and 2.28) (Table 2.9).

### 2.6.5 Delayed Fission Neutrons

Delayed particle emission occurs with both neutron-deficient and neutron-rich nuclei. Proton emission was observed for the first time in 1962, while delayed neutron emission being seen initially in 1939 by R.O. Meyer and Wang. In 1939, Bohr and Wheeler investigated the possible origin of these delayed neutrons and concluded that this phenomenon occurs upon $\beta^{-}$decay of certain fragments. It was long thought that only 6 delayed neutron precursors existed, until in 1953 A. C. Pappas reported the existence of numerous periods of delayed neutrons. Nevertheless, to this day delayed neutrons continue to be widely grouped under 6 families. Maria Mayer was the first person to note the effects of closed (completely filled) neutron shells on the emission of delayed neutrons. Subsequent studies showed that the precursors are frequently located far from regions of closed neutron shells. The greater the neutron charge of a fission fragment, the further it is from stability, and the weaker the neutron binding energy, $B_{n}$, and conversely, the greater the energy $Q_{\beta}$ between two isobaric isotopes. At a certain distance from stability, the following may be found:
Table 2.9 Prompt fission gamma spectrum and energy spectrum

| Energy [MeV] | 0.5 | 1 | 1.5 | 2 | 2.5 | 3 | 3.5 | 4 | 4.5 | 5 | 5.5 | 6 | 6.5 | total |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $n(E)[$ gamma/fission $]$ | 3.1 | 1.9 | 0.84 | 0.55 | 0.29 | 0.15 | 0.062 | 0.065 | 0.024 | 0.019 | 0.017 | 0.007 | 0.004 | 7.028 |
| $m(E)[\mathrm{MeV} /$ /fission $]$ | 1.55 | 1.9 | 1.26 | 1.1 | 0.725 | 0.45 | 0.217 | 0.26 | 0.108 | 0.095 | 0.0935 | 0.042 | 0.026 | 7.8265 |

Table 2.10 Number of delayed neutrons per fission for some fissile isotopes

| Fissile nucleus | Number of delayed neutrons per fission |
| :--- | :--- |
| ${ }_{92}^{235} U$ | 0.0158 |
| ${ }_{92}^{233} U$ | 0.0066 |
| 239 <br> ${ }_{94}^{238} \mathrm{Pu}$ <br> 92 | 0.0061 |

$$
Q_{\beta}-B_{n} \geq 0
$$

The $\beta^{-}$radioactivity of an isotope ${ }_{Z}^{A} X$ containing $A-Z$ neutrons can produce excited states ${ }_{Z+1}^{A} Y^{*}$ holding $A-(Z+1)$ neutrons. If the level of excitation attained is greater than the binding energy, $B_{n}$, there may be de-excitation to the ground state ${ }_{Z+1}^{A-1} Y^{*}$ with the emission of a neutron. In this case, the nucleus ${ }_{Z}^{A} X$ is called a delayed neutron precursor while the nucleus ${ }_{Z+1}^{A} Y^{*}$ is termed a delayed neutron emitter. The delayed neutron spectrum is mainly continuous, but with some fairly pronounced peaks at around 0.2 MeV . It should be noted that delayed neutrons are emitted at a lower energy level (between 0.2 and 0.6 MeV ) than prompt neutrons. Delayed neutrons created through $\beta^{-}, n$ decay (or "neutron decay") from extremely neutronrich radioactive fission products. They are quantified in terms of the fission event that created the fission products in question. Around $1 \%$ of the neutrons emitted following fission are delayed neutrons.

Although they occur in low numbers, these neutrons are essential for reactor control. If there were only prompt neutrons, the reactor would become uncontrollable since divergence would be explosive. The number of delayed neutrons per fission (absolute delayed neutrons yield) depends on the fissile nucleus in question. The absolute delayed neutrons yield is directly correlated with the yield of delayed neutrons by fission of the precursor.

The greater the number of delayed neutrons per fission (see Table 2.10), the "slacker" ${ }^{17}$ the fuel containing the fissioning nucleus in question, in other words the easier to manage. Fuel containing heavy nuclei with small numbers of delayed neutrons per fission will be highly reactive in the event of reactivity accidents and thus more difficult to control. Consequently, the Natural Uranium and Graphite-Gas ( $U N G G$ in French) reactors containing little ${ }_{92}^{235} U$ and a great deal of ${ }_{92}^{238} U$ are easier to control than fast-neutron reactors containing large quantities of ${ }_{94}^{239} \mathrm{Pu}$ (Tables 2.11, 2.12 and 2.13).

The delayed neutron fraction, $\beta$, denotes the number of delayed neutrons divided by the total number of neutrons emitted. $\beta$ is often expressed in pcm (pour cent mille). The delayed neutron fraction depends on the fissioning isotope and on the incident neutron energy (Table 2.14 gives no data for non-fissile isotopes in thermal spectrum).

[^44]Table 2.11 Delayed neutrons for ${ }_{92}^{235} U$

| Group | Period [s] | Abundance [\%] | Total neutrons per fission |
| :--- | :--- | :--- | :--- |
| 1 | 55.7 | 3.3 | 0.00052 |
| 2 | 22.7 | 21.9 | 0.00346 |
| 3 | 6.2 | 19.6 | 0.00310 |
| 4 | 2.3 | 39.5 | 0.00624 |
| 5 | 0.61 | 11.5 | 0.00182 |
| 6 | 0.230 | 4.2 | 0.00066 |
| Total |  | $100 \%$ | 0.0158 |

Table 2.12 Delayed neutrons for ${ }_{92}^{233} U$

| Group | Period $[\mathrm{s}]$ | Abundance [\%] | Total neutrons per fission |
| :--- | :--- | :--- | :--- |
| 1 | 55.0 | 8.6 | 0.00057 |
| 2 | 20.57 | 29.9 | 0.00197 |
| 3 | 5.0 | 25.2 | 0.00166 |
| 4 | 2.13 | 27.8 | 0.00184 |
| 5 | 0.615 | 5.1 | 0.00034 |
| 6 | 0.277 | 3.4 | 0.00022 |
| Total |  | $100 \%$ | 0.00660 |

Table 2.13 Delayed neutrons for ${ }_{94}^{239} P u$

| Group | Period [s] | Abundance [\%] | Total neutrons per fission |
| :--- | :--- | :--- | :--- |
| 1 | 54.3 | 3.5 | 0.00021 |
| 2 | 23.0 | 29.8 | 0.00182 |
| 3 | 5.60 | 21.1 | 0.00129 |
| 4 | 2.13 | 32.6 | 0.00199 |
| 5 | 0.618 | 8.6 | 0.00052 |
| 6 | 0.257 | 3.4 | 0.00027 |
| Total |  | $100 \%$ | 0.00610 |

Table 2.14 Delayed neutron fractions for major fissile systems

| $\beta(\mathrm{pcm})$ | Fast | Thermal |
| :--- | :--- | :--- |
| ${ }_{92}^{233} U$ | $270 \pm 20$ | $264 \pm 20$ |
| ${ }_{92}^{235} U$ | $650 \pm 30$ | $650 \pm 30$ |
| ${ }_{92}^{238} U$ | $1570 \pm 120$ | - |
| ${ }_{92}^{239} \mathrm{Pu}$ | $210 \pm 20$ | $210 \pm 20$ |
| ${ }_{94}^{240} \mathrm{Pu}$ | $260 \pm 30$ | - |
| ${ }_{94}^{232} \mathrm{Th}$ | $2200 \pm ?$ | - |

Table 2.15 Precursor groups for ${ }_{92}^{235} U$

| Precursor | Period (s) | Neutron energy <br> $(\mathrm{MeV})$ | Number of delayed <br> neutrons per fission <br> neutron $\left(\beta_{i}\right)$ |
| :--- | :--- | :--- | :--- |
| ${ }_{35}^{87} \mathrm{Br}$ to ${ }_{36}^{87} \mathrm{Kr}$ | 55.6 | 0.25 | 0.00026 |
| ${ }_{53}^{137}$ I to ${ }_{54}^{137} \mathrm{Xe}$ | 22.0 | 0.46 | 0.00170 |
| ${ }_{35}^{89} \mathrm{Br}$ to ${ }_{35}^{91} \mathrm{Br}$ | 4.51 | 0.40 | 0.0021 |
| ${ }_{53}^{139}$ or ${ }_{51}^{135} \mathrm{Sb}$ | 1.52 | 0.45 | 0.0024 |
| ${ }_{51}^{137} \mathrm{Sb}$ | 0.43 | 0.42 | 0.00084 |
| 85 As | 0.05 | - | 0.00025 |

Delayed neutrons are grouped together by family according to the fission products of similar period by which they are produced. The number of delayed neutron groups has been optimized for the study of reactor kinetics to 6 groups (not to be confused with energy groups!). The percentage thus corresponds to weighting of the fission yields of the isotopes included in these families. The main precursors and the average energy of the emitted neutrons are given in Table 2.15. It may be seen that this energy is far less than the mean fission energy ( 2 MeV ). Consequently, delayed neutrons are not so important inside the reactor, and in particular, they are practically incapable of causing fission in fast isotopes such as ${ }_{92}^{238} U$ which have threshold fission cross sections. Both the periods and abundance of delayed neutron groups are relatively unaffected by the energy of neutrons causing fission. This effect is of secondary importance in relation to the fissile nucleus effect.

### 2.7 Fission Products Resulting from Fission

Fission products are created statistically as a percentage of the fission yield, which has a highly characteristic double-humped curve (the so-called camelback-though not a dromedary back-curve, as everyone knows!) peculiar to each heavy fissile nucleus. The sum of the yields is normalized to 2 (since two nuclei are produced). The fission yield of a fission product depends on the fissioning isotope and on the energy of the incident particle. Nuclear libraries provide three yield values for each fissile system: the so-called high-energy yield for neutrons at 14 MeV , a fast yield for neutrons at 400 keV , and a thermal yield for neutrons having a Maxwellian distribution. The two peaks in the curve are centered around the neighboring masses of 95 and 140 , whereas a single peak would be centered approximately around half the mass number of the fissile isotope.

This asymmetry is due to the fact that the fission products tend to be distributed around the magic numbers of nucleons (Reuss 1987, p58), (GA, Vol. 1 1967, p132). Whetstone proposed a simple empirical model to account for the fact that for fission products of comparable mass, the lightest fragment receives the highest excitation

Fig. 2.29 Total chain yield per fission of ${ }_{92}^{235} \mathrm{U}$ as a function of mass number, after Reactor Physics Constants ANL-5800. Circle: thermal neutrons triangle: neutrons at 14 MeV

energy (Nuclear Structure 1960, p865). This idea is based upon the position of the fracture of the deformed compound nucleus: Whetstone defined a probability of rupture that is symmetrically dependent on the distance from the rupture.

For an actual reactor, the yields are weighted by the fast and thermal reaction rates with a cut-off energy (generally 0.625 eV ), enabling the thermal part be considered as corresponding to a Maxwell spectrum, while the fast part corresponds to a fast and epithermal spectrum. To simplify, the thermal yield provides a good approximation of the yield of a fission product in a $P W R$ reactor. The yields produced by a high-energy neutron $(14 \mathrm{MeV})$ are of the same order of magnitude as those produced at low energy, except in the middle of the hump, where the divergences are significant and can reach a coefficient of 100 . At high energy levels, the number of neutrons emitted per fission increases. Note that certain fissile systems such as ${ }_{92}^{238} U$ only fission by means of fast neutrons (since the fission cross section is a threshold cross section). Figure 2.29 presents the total chain yield as a function of mass number. It may be seen that the maximum yield is of the order of $6.4 \%$ for mass numbers in the vicinity of 95 (first hump) or 137 (second hump).


Fig. 2.30 Whetstone fission model. Where fission occurs at the scission point, most probably midway between the nuclei, asymmetric distribution of mass occurs since the fragments tend to conform to the magic number rule for nucleons, thus one light fragment and one heavy fragment. If scission occurs near the lighter nucleus, the heavier nucleus will be that most excited by the deformation energy, and the masses of the two fragments will differ greatly; more equitable distribution of masses signifies scission near the heavy fragment, in which case the "intermediate" mass will make the light fragment heavier, resulting in this case in the light fragment being the most excited

This is why it was the isotope ${ }_{56}^{137} B a$ that enabled the discovery of fission, since it is produced in greater quantities (Fig. 2.30).

### 2.7.1 Direct Yield of an Isotope

The term direct yield (or independent yield) denotes the percentage of an isotope created directly by fission following the emission of prompt neutrons, but prior to the emission of delayed neutrons. This is a relatively subjective notion, since it is difficult for researchers to ensure that a given isotope is not the product of the extremely rapid decay of a "highly-volatile" transient parent entity. Regardless, independent decay thus does not take into account the potential formation of the isotope by parent entities that might have produced it through radioactivity. Not all directly yields have necessarily been measured and yields are generally normalized to the yield of ${ }_{56}^{140} \mathrm{Ba}$ for thermal fission of ${ }_{92}^{235} U+n$, i.e. $6.44 \%$. The independent yield of an isotope of mass number $A$, atomic number $Z$, and isomeric state $I$ is written as $y(A, Z, I)$.

### 2.7.2 Total Chain Yield

The total isobaric chain yield $Y(A)$ is defined as the sum of the different independent yields of fission products having the same mass number $A$. The total chain yield of a radioactive isotope is frequently noted alongside the name of a radioactive isotope, which indicates that it is the last isotope created directly by fission in the mass number in question. The maximum value attained is of the order of $7 \%$. If $f(A, Z)$ is the independent yield fraction of all isomers of $(A, Z)$ and $R(A, Z, I)$ is the yield ratio of the isomer in question, we have the following closure laws:

$$
\left\{\begin{array} { l l } 
{ \forall A , } & { \sum _ { Z } f ( A , Z ) = 1 } \\
{ \forall ( A , Z ) , } & { \sum _ { I } R ( A , Z , I ) = 1 }
\end{array} \quad \left\{\begin{array}{l}
\forall A, \quad \sum_{Z, I} y(A, Z, I)=Y(A) \\
\sum_{A} Y(A)=2
\end{array}\right.\right.
$$

The value of these formulae stems from the fact that most of the radioactivity of fission products is of the type $\beta^{+}$or $\beta^{-}$and thus conserves the relevant mass numbers during successive decays (with the exception of $\beta^{-}$decays of delayed neutron precursors). It may therefore be assumed with relatively little risk of error that the fission product chains are distinct in terms of mass number. These closure laws are extremely useful as a complement to any theoretical models that provide independent yields for unmeasured isotopes. These models, such as the Wahl ${ }^{18}$ model for example, enable the independent yield to be calculated using the formula:

$$
f(A, Z)=\frac{1}{2} F(A, Z) N(A)\left\{\operatorname{erf}\left(\frac{Z-Z_{p}(A)+0,5}{\sigma_{z} \sqrt{2}}\right)-\operatorname{erf}\left(\frac{Z-Z_{p}(A)-0,5}{\sigma_{z} \sqrt{2}}\right)\right\}
$$

where $N(A)$ is a normalization coefficient allowing verification of normalization to 1 of the independent yields, $F(A, Z)$ represents the even-odd effect, and $Z_{p}(A)$ and $\sigma_{z}$ are respectively the mean value and standard deviation of a Gaussian distribution that does not include the odd-even effect. The cumulative chain yield may be modeled using 5 Gaussian distributions ${ }^{19}$ (two for each peak and one for the symmetrical central part of the fission):

[^45]\[

$$
\begin{aligned}
Y(A)= & \frac{N_{1}}{\sigma_{1} \sqrt{2 \pi}}\left(e^{-\left(A-\bar{A}-D_{1}\right)^{2} / 2 \sigma_{1}^{2}}+e^{-\left(A-\bar{A}+D_{1}\right)^{2} / 2 \sigma_{1}^{2}}\right) \\
& +\frac{N_{2}}{\sigma_{2} \sqrt{2 \pi}}\left(e^{-\left(A-\bar{A}-D_{2}\right)^{2} / 2 \sigma_{2}^{2}}+e^{-\left(A-\bar{A}+D_{2}\right)^{2} / 2 \sigma_{2}^{2}}\right)+\frac{N_{3}}{\sigma_{3} \sqrt{2 \pi}} e^{-(A-\bar{A})^{2} / 2 \sigma_{3}^{2}}
\end{aligned}
$$
\]

where $N_{i}$ is the normalization factor of the $i$ th Gaussian function and $\sigma_{i}$ is its standard deviation, $\bar{A}$ is the mean mass of the distribution, and $D_{i}$ is the deviation of the peak in Gaussian function from the mean value $\bar{A}$. Normalization of chain yields to 2 implies that $N_{3}=2\left(1-N_{1}-N_{2}\right)$.

### 2.7.3 Cumulative Yield of an Isotope

The cumulative yield is defined as the probability of appearance of an isotope formed either directly through fission, or by radioactive decay of its parent atoms in the decay chain. It is thus the total number of atoms of fission product accumulated over time following fission excluding any radioactivity of the latter. This assumes instantaneous decay of all parents in the isotope for which we are seeking the cumulative yield. The cumulative yield of a given isotope is always less than the chain yield of its mass number since isotopes of the same mass not contained in the chain of its parents may be created directly by fission and are naturally not counted in the cumulative figure for the isotope in question. Note that because of the presence of isomers, which may be created directly by fission, the limited yield of the last isotope in the chain may also be lower than the chain yield (in which the isomer is counted in the same way as the fundamental isotope), when the isomer decays not only to its fundamental state but also to an isotope of different mass number (e.g. $\alpha$ decay). Cumulative yields are used to calculate the residual power of all fission products.

### 2.7.4 Slowing Down of Fission Products in Matter

During fission, the fragments acquire strong acceleration due to Coulomb repulsion between the two nuclei. As a first approximation, it may be considered that their kinetic energies are inversely proportional to their mass at speeds of the order of $10,000 \mathrm{~km} / \mathrm{s}$. For incident neutrons of energy below 2 MeV , fission is overwhelmingly isotropic. This is no longer the case above this level, where forward scattering is preponderant. Given the loss of electrons, the effective charge of the fragments is around $+20 e$. Slowing down thus occurs primarily through different ionizations throughout their trajectory, during which their electronic cloud fills up and the atom finally becomes neutral (GA Vol. 1 1967, p13).

# Chapter 3 <br> Interaction of Electromagnetic Radiation and Charged Particles with Matter 


#### Abstract

All nuclear reactions are associated with the emission of radiation. This radiation contributes in part to the release of nuclear energy by interacting with materials in the reactor core, and more generally, poses problems of radioprotection. Similarly, a large number of particles is created during operation of the reactor, in particular, charged particles such as $\alpha$ particles, as well as electrons and positrons as a result of $\beta$ radioactivity. All of these particles interact with matter and release energy that contributes to the thermal balance of the pile. They also pose radioprotection problems for staff and can damage the reactor structures through the cumulative effects of collision. In this chapter, we examine the fundamentals needed to understand the phenomena of interaction between charged particles and matter. (Baur 1985; Berthelot 1956; Born 1971; Brasseur 1945; Cohen-Tannoudji et al. 1988; Delacroix et al. 2006; Filippi 1965; Herzberg 1991; Hine and Brownell 1956; Lawson 1977; Métivier 2006; Shultis and Faw 2000; Sigmund 2008; Sharpe and Taylor 1958, p. 103).


### 3.1 Electromagnetic Radiation

(Loudon 2000)
The frequency range of electromagnetic waves varies greatly.
Figure 3.1 gives a breakdown of the spectrum into radio waves (wavelength 30 km to 1 mm ), followed by submillimeter, infrared (Déribéré 1954), visible and ultraviolet radiation, and then x-rays (Brasseur 1945) and $\gamma$ rays. These different names refer to a single physical phenomenon: electromagnetic radiation Radio waves are themselves grouped according to different applications such as television, radar, etc. We generally speak of frequency (Hertz) for low energy levels, but of electronvolts ( eV ) for higher energies. Electromagnetic waves may be envisaged in the form of either waves (having a wavelength $\lambda$ ) or corpuscles (photons of energy $h v$ ).


Fig. 3.1 Types of electromagnetic radiation by wavelength range and energy

At low energy levels (radio waves), only the wave function is of interest. At high energies (x-rays and beyond), the particle function (corpuscular properties) is crucial. The frequency characterizing a wave is given by: $v_{\left[\mathrm{s}^{-1}\right]}=c / \lambda$ where $c$ is the speed of light in a vacuum. The energy of a photon is given by $E_{[J]}=h v=m c^{2}$. The mass thus defined is in fact an equivalent mass since photons have no discernible mass.

### 3.2 X-radiation

(Boutaric 1948; Peaslee and Mueller 1955, p. 104)
Analysis of energetic photons began at the end of the nineteenth century. Progress with the Ruhmkorff coil, invented by German engineer Heinrich D. Ruhmkorff (1803-1877), and the generation of high-voltage discharges (around $20,000 \mathrm{~V}$ ), enabled high-speed electron currents to be produced in Crookes tubes, invented by Sir William Crookes (1832-1919). Thanks to the use of increasingly efficient vacuum tubes, Julius Plücker (1801-1868) was able to discover in 1858 that the light appearing on discharge disappears at very low pressures since collisions no longer occur between electrons and air molecules. In 1895, Wilhelm Röntgen (1845-1923) succeeded in bombarding the target anode of his vacuum tube with extremely high energies (Photos 3.1, 3.2).

He detected highly penetrative radiation which he dubbed $x$-rays (" $x$ " for "unknown"), the attenuation of which by dense substances enabled him to obtain the first radiograms. A radiographic image taken of his wife Bertha's hand enjoyed phenomenal success and very quickly made the rounds throughout Europe. An enormous opaque ring may clearly be made out on one of Mrs. Röntgen's fingers. Following the discovery of x-rays, many studies conducted to analyze their electromagnetic characteristics. Charles Barkla (1877-1944), winner of the Nobel Prize in Physics in 1917, showed in 1905 that they were polarizable ${ }^{1}$ (Brasseur 1945, p. 12).

[^46]

Photo 3.1 Wilhelm Röntgen (left) is celebrated in Germany as the first winner of the Nobel Prize in Physics in 1901, as indicated in the commemorative stamp issued by the West German Post Office (Public domain and the Marguet collection).


Photo 3.2 The famous radiograph of Mrs. Röntgen's hand (Public domain)

Studies in 1908 by B. Walter and Robert Pohl, followed by those of Koch and finally Arnold Sommerfeld, established the possibility of deflecting x-rays through a slit, thereby demonstrating the wave character of this form of radiation. In June 1912, Walter Freidrich, Paul Knipping and Max Von Laue (1879-1960) provided irrefutable proof [using a device described in Brasseur (1945, p. 15)] of the diffraction of x-rays by crystals, thus opening the way for modern crystallography that allows the study of periodic networks. William L. Bragg (1890-1971) showed that on the basis of Von Laue's analysis, the condition of diffraction is written as a function of:

- $\theta$, the angle of the incident beam and of the diffracted beam at maximum intensity,
- $d$, the reticular distance,
$-\lambda$, the wavelength of $x$-rays,
with $\theta / 2$ being the glancing angle, i.e. the complement of the angle of incidence (Brasseur 1945, p. 42; Squires 1996; p. 33; Valentin 1982a, b, p. 33). In Fig. 3.2, $A O$ represents the incident neutron wave vector and $A B$ the scattered neutron wave vector. Since the collision is elastic, $A O=A B . B O$ is the vector perpendicular to the lattice of crystal planes such that $B O=2 \pi n / d$ where $n$ is an integer.

$$
\begin{equation*}
\text { Bragg's law : } \quad n \lambda=2 d \sin \frac{\theta}{2} \tag{3.1}
\end{equation*}
$$

This law is also valid for the diffusion of neutrons by a crystal.
The principle of radiography is based upon the exponential absorption of x-rays, the attenuation coefficient of which increases with the density of the matter through which they pass (Brasseur 1945, p. 31). X-ray imaging enjoyed massive success and in the First World War in 1914-1918, Marie Curie created a military ambulance corps equipped with x-ray equipment allowing radiography to be performed near the battlefield. Her daughter, Irène Joliot-Curie, worked as an assistant for the use of this device (Radvanyi 2005). In the 1950s, extremely detailed treatises on electrotherapy were published for the attention of the medical professions (Delherm 1951).

One of the principal ways of creating x-rays is through braking radiation or Bremsstrahlung (in German). The trajectory of the negative electron curves due to Coulomb's force of attraction of positively-charged protons and the electron is abruptly slowed down. Loss of energy by the electron is compensated by the emission of an x-photon, in the same way as a catapult releases its stone when

Fig. 3.2 Coherent elastic diffusion in the reciprocal plane of the wave vectors


Fig. 3.3 Slowing-down of an electron by the nucleus with emission of an x-ray via Bremsstrahlung


Scattered electron of energy $E^{\prime}<E$
the rotary movement is halted. The emission spectrum is continuous but is limited by the kinetic energy of incident electrons (Fig. 3.3).

At low energy, the measurable spectrum is limited by the phenomenon of autoabsorption of the target (neighboring atoms absorb the least energetic $X$ photons). It is possible for the interaction of an electron (or an $\alpha$ particle) to excite an electron in the target without detaching it. In this event we have an excited electron in the electron cloud that de-excites towards the ground state by emitting a photon. This photon, if situated at the right wave length (in other words the atom is sufficiently heavy and the electron belongs to a sufficiently deep shell), will be an x-ray. These emissions were analyzed by Henry G. Moseley (1887-1915), who in 1913 studied the correspondence between emitted frequencies and atomic number $Z$ (Renault 1948, p. 85; Jouguet 1964, p. 54) and then quantified. They produce x-rays characteristic of the target that are precisely described in the Bohr-Sommerfeld theory. The most energetic photons-which we shall call $\gamma$ rays, using the term x-rays for electron emission-are produced by de-excitation of the excited nuclei which return to their ground state by emitting nuclear photons. It is thus possible to obtain a cascade of photons passing through intermediate energy levels where the energy of the nucleus is far higher than that of its ground state. Indeed, x-rays are used in a host of applications in the field of metrology [non-destructive control testing, spectroscopy (Turpain 1913, p. 77), imaging, etc.]. ${ }^{2}$

### 3.3 Interaction of Photons with Matter

(Baur 1985; Berthelot 1956; Cabannes 1929; Delacroix et al. 2006; Filippi 1965; Harrison 1958; Lilley 2001, p. 136; Métivier 2006; Pollard and Davidson 1956; Semat 1955; Thorre et al. 1999).

[^47]
### 3.3.1 Attenuation of a Photon Beam

(Goldstein 1959, p. 140)
As a monokinetic beam of photons passes through matter of a certain thickness, an exponential loss of energy (illuminance) occurs. Energetic illuminance is defined by the following formula:

$$
I_{\left[\mathrm{W} / \mathrm{m}^{2}\right]}=\frac{d \Phi}{d s}
$$

where $\Phi$ is the energy flux in Watt and $d s$ the area of the interposed screen. The attenuated rays crossing in a straight line (these are occasionally referred to as ballistic rays, indicating photons that do not undergo shock) may be distinguished from scattered rays that have undergone collision. It can be seen that backwards diffusion is possible (this phenomenon is known as backscattering). Because of attenuation, the energy transmitted behind a screen is lower than the incident energy. The difference in energy is that transferred to the interposed screen (Fig. 3.4).

If the $x$-axis origin is placed at the start of the screen, photon attenuation may be written as:

$$
I_{\left[\mathrm{W} / \mathrm{m}^{2}\right]}=I_{0} e^{-\mu(E) \cdot x}
$$

The coefficient $\mu$ is known as the linear attenuation coefficient $\left[\right.$ in $\mathrm{m}^{-1}$ ] and depends on the type of matter being crossed and the energy of the photons in question. The inverse value, $1 / \mu$, is sometimes referred to as the mean free path of photons in matter. Attenuation is often presented in the form of mass attenuation using the density of the matter crossed by the photons:


Fig. 3.4 Attenuation of energy of photons on passing through a screen

$$
\begin{equation*}
\text { Linear attenuation of photons : } I_{\left[\mathrm{W} / \mathrm{m}^{2}\right]}=I_{0} e^{-\frac{\mu(E) \cdot}{\rho} \cdot \rho x} \tag{3.2}
\end{equation*}
$$

This law is known as the Beer-Lambert-Bouguer law by direct analogy with the attenuation of a monochromatic beam in a liquid at concentration $c$ and having an absorption coefficient $\alpha$ (Fig. 3.5):

$$
I_{1\left[\mathrm{~W} / \mathrm{m}^{2}\right]}=I_{0} e^{-\alpha c \ell}
$$

The same law as that governing irradiance applies to the number of photons: $N=N_{0} e^{-\mu(E) \cdot x}$.

It can be shown experimentally that the denser the matter crossed, the greater the degree of attenuation. Similarly, the selective absorption of particular wavelengths by different chemical bodies forms the underlying principle of atomic absorption spectrometry (Pinta et al. 1979), which for example allows rapid analysis of the impurities present in a given sample of gas (Turpain 1913, p. 79). The protective screen industry regularly uses the concept of the half-value layer (HVL), which is the thickness of a screen at which the number of photons transmitted is reduced by half. These values are energy-dependent, and for information, Table 3.1 provides some values for standard materials and photons at 1 MeV :


Fig. 3.5 Beer-Lambert-Bouguer law (source: Wikipedia)

Table 3.1 Efficiency of gamma-radiation shielding materials

|  | Water | Concrete | Iron | Lead |
| :--- | :--- | :--- | :--- | :---: |
| Density $\rho\left[\mathrm{g} / \mathrm{cm}^{3}\right]$ | 1.00 | 2.30 | 7.85 | 11.30 |
| Attenuation coefficient $\mu\left[\mathrm{cm}^{-1}\right]$ | 0.07 | 0.15 | 0.47 | 0.79 |
| HVL $[\mathrm{cm}]$ | 9.90 | 4.62 | 1.47 | 0.88 |

### 3.3.2 Photon Transport

(Goldstein 1959, p. 159)
If we now examine photons moving in different directions and at different energies, we must first of all define (Duderstadt and Martin 1979) the intensity of the photons as the product of the energy $h v$ and the photon flux at speed $c$ and concentration $n(\vec{r}, E, \vec{\Omega}, t)$ :

$$
I(\vec{r}, \vec{\Omega}, t)=h v n(\vec{r}, E, \vec{\Omega}, t)
$$

The equation governing photon transport, known as the Boltzmann equation, is written:
$\frac{1}{c} \frac{\partial I(\vec{r}, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad} I}(\vec{r}, \vec{\Omega}, t)=\rho(\vec{r}, t)[-\kappa(\vec{r}, \vec{\Omega}, t) I(\vec{r}, \vec{\Omega}, t)+\varepsilon(\vec{r}, \vec{\Omega}, t)]$
where:
$\rho(\vec{r}, t)$ is the density of the medium crossed
$\kappa(\vec{r}, \vec{\Omega}, t)$ is the photon absorption coefficient, which depends on the nature of the medium crossed
$\varepsilon(\vec{r}, \vec{\Omega}, t)$ is the emission coefficient, which depends on the nature of the medium crossed

At thermodynamic equilibrium at temperature $T$, the black-body radiation law (Planck's formula) gives the ratio between emission and absorption:

$$
B_{v}=\frac{\varepsilon}{\kappa}=\frac{2 h v^{3}}{c^{2}} \frac{1}{e^{\frac{h v}{k t}}-1}
$$

If we take into account elastic scattering (Rayleigh-Thomson scattering) for the re-emission of photons at the same frequency, using the ratio of the absorption cross-section to the total cross-section (absorption + diffusion), we may write:

$$
\begin{aligned}
\frac{1}{c} \frac{\partial I(\vec{r}, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad} I(\vec{r}, \vec{\Omega}, t)=} & \rho(\vec{r}, t) \kappa(\vec{r}, \vec{\Omega}, t)\left[-I(\vec{r}, \vec{\Omega}, t)+\frac{\sigma_{a b s}}{\sigma_{t o t}} B_{v}\right. \\
& \left.+\left(1-\frac{\sigma_{a b s}}{\sigma_{t o t}}\right) \int \frac{d \Omega}{4 \pi} I(\vec{r}, \vec{\Omega}, t)\right]
\end{aligned}
$$

The integral for the frequencies in this equation leads to an equation very similar to the equation for neutron transport in one energy group.

### 3.3.3 Rayleigh-Thomson Scattering

(Loudon 2000, p. 339; Shultis and Faw 2000, p. 42).
This is the simplest case of interaction in which a photon collides with matter without loss of energy. During this type of scattering, which is also called coherent diffusion, the photons excite electrons, which oscillate and re-emit photons at the same energy as the incident photons. This phenomenon is known as elastic diffusion without energy transfer. It is important at low energies although such diffusion is generally disregarded in favor of the other interactions of photons. The differential cross section as a function of the diffusion angle is given by the Thomson formula (Hine and Brownell 1956, p. 55):

$$
\frac{d \sigma(\theta)}{d \Omega}=\frac{r_{e}^{2}}{2}\left(1+\cos ^{2} \theta\right)=\frac{e^{4}}{2 m_{e}^{2} c^{4}}\left(1+\cos ^{2} \theta\right)
$$

where $r_{e}$ is the electron radius $\left(2.817938 \times 10^{-14} \mathrm{~m}\right)$. This formula is valid for a free electron. For a bound electron, the moment of recoil, $q$, may be transferred to $Z$ electrons without energy absorption, but the formula is corrected by a multiplicative term dictated by the atomic number of the target. The correction coefficient may be obtained by means of complex quantum-electrodynamics calculations, out of the scope of this book:

$$
\frac{d \sigma(\theta)}{d \Omega}=\frac{r_{e}^{2}}{2}\left(1+\cos ^{2} \theta\right) F(q, Z)
$$

### 3.3.4 Photoelectric Effect

Antoine Becquerel, the grandfather of Henri Becquerel, was apparently the first person to have observed (in 1839) electrical current resulting from the action of light [(Zworykin and Ramberg 1953, p. 1), in which he is, however, confounded with his son, Edmond]. He noted that a blue light resulted in a stronger current between a pair of electrodes placed in electrolyte than did a yellow or a red light. He presented this photovoltaic effect to the French Science Academy in late 1839. In

1887, while working on the production of sparks and electrical arcs, Heinrich Hertz ${ }^{3}$ (1857-1894) noticed that production was in fact facilitated if the cathode was bathed in ultraviolet light. He thus devised the following experiment to understand this phenomenon. A fine sheet of zinc is placed on an experimental device comprising an electroscope and then illuminated with like resulting either from an electrical arc or from a mercury-vapor lamp rich in ultraviolet radiation.

It may be seen that if the electroscope is negatively charged and the zinc sheet then lit up, the electroscope discharges continuously and rapidly, indicating that electrons are expelled from the metal by the ultraviolet rays. A positive charge then builds up in the zinc sheet, which discharges the electroscope. Conversely, if the

[^48]

Heinrich Hertz
electroscope is positively charged, the discharge no longer occurs since the electrons created by the process are attracted to the electroscope. Further, if a glass that absorbs the ultraviolet radiation in light is interposed, discharge no longer occurs. The logical conclusion is that when adequately lit, the zinc sheet emits electrons. This phenomenon is known as the photoelectric effect. If a light source strikes a metal plate, the electromagnetic waves detach electrons from the metal which may then be attracted by a positively charged plate (anode), thereby creating an electric current (Figs. 3.6 and 3.7).

It may be seen experimentally that the frequency of the radiation must exceed a certain level in order to initiate the photoelectric current. Even if the position of the anode becomes slightly negative, current is measurable, but decreases in accordance with the negative value at the anode. When the current is extinguished, we may deduce the maximum kinetic energy carried by the electrons (Cagnac and Pebay-Peyroula 1995, p. 7). The photoelectric current occurs quasi-instantaneously when the light source is switched on and the maximum kinetic energy of the electrons does not vary with the intensity of the light. Classical electromagnetic theory cannot account for these phenomena, since if it were the wave that excites an electron in order to detach it from the metal, this phenomenon would occur at all wavelengths if sufficient time were allowed.


Fig. 3.6 Lamp switched off: no electrons produced


Fig. 3.7 Lamp switched on: electrons produced by zinc


Further, the kinetic energy of the electrons should depend upon the intensity of the wave, but this is not what happens in experiments. Albert Einstein accounted for the photoelectric effect positing the existence of a particle, the photon, ${ }^{4}$ a sort of "grain of light" that transports the energy of the light beam (Bergia 2004, p. 31). This particle also possesses wave qualities, as part of its dual particle/wave nature. In order to overcome the dead-end posed by the problem of the photoelectric effect, he proposed in 1905 that Plank's quanta notion be applied to light.

A wave train with an extremely high frequency has particle properties, in other words particle of energy, $h v$. As soon as the energy of a photon is able to overcome the binding energy $W$ responsible for the bond between the electron and the atomic nucleus, the electron is ejected with kinetic energy $T_{e^{-}}=h v-W$. If the intensity of the light increases, so too does the number of detached electrons, but not their kinetic energy, since the energy of photons is fixed (it is in fact the number of photons that increases with intensity). The device shown in Fig. 3.8 enables either positive or negative current to be applied. A negative countercurrent, $-V_{0}$, independent of the frequency of the light must be used to cancel out the photoelectric effect induced when the photocathode is lit. With more negative currents, the electrode repels the electrons. The effective cross section of the photoelectric effect, usually denoted $\tau$, presents discontinuity at each level of binding energy in the electron shell up to the

[^49]Fig. 3.8 Electrical device to measure the stopping potential

most tightly bound level, $K$, beyond which the cross section varies inversely with the cube of the energy of the photon $1 /(h v)^{3}$ (Figs. 3.9 and 3.10).

A photon with sufficient energy can expel an electron by transferring to it the kinetic energy equal to the difference between the energy of the photon $h v$ and the binding energy of the outermost electron. Following the collision, the photon disappears after transferring all of its energy. For conservation of the impulse, the pattern to which the electron undergoing collision belongs participates by carrying away the remainder of the impulse [this also means that complete disappearance of a photon that projects a free electron is physically impossible, and there is inevitably a Compton effect (GA Vol. 1 1967, p. 85)]. The photoelectric phenomenon is especially likely with photons of energy less than 100 keV . The probability of interaction [linear attenuation coefficient (Hine and Brownell 1956, p. 53) due to photoelectric effect $\tau$ ] is given by the empirical law of William Henry Bragg $(1862-1942)^{5}$ and S.E. Peirce (Cahen and Treille 1963; Shultis and Faw 2000, p. 44):

$$
\frac{\tau}{\rho} \approx C s t \frac{Z^{3}}{A} \frac{1}{(h v)^{2,8}}
$$

[^50]Fig. 3.9 Ejection of an electron from electron cloud by a photon


Fig. 3.10 Re-arrangement of electron cloud


This formula shows that the photoelectric effect is enhanced in media with a high Z (such as metals), but that it decreases considerably with energy. Expulsion of an electron from the $K$ shell results in rearrangement of the electrons and in the consequent emission of an $X$ photon by fluorescence in what is known as the Auger effect (Mayo 1998, p. 285). The expelled electron is termed the Auger electron. Photoelectrons are emitted in all directions but principally forwards at high photon energies. Einstein's original approach to the photoelectric effect won him the Nobel Prize in 1921 "for his services to theoretical physics, and especially for his discovery of the law of the photoelectric effect". More or less deterministic models can be used to obtain laws of the effective cross section of the photoelectric effect, such as Heitler's law (Baur 1985, p. 71), which describes the non-relativistic contribution of electrons in the $K$ shell for photons at energies below 0.5 MeV .

### 3.3.5 Compton Effect

When waves are reflected or diffracted by obstacles, no change is expected in either wavelength or frequency, although there may possibly be some variation in intensity. However, if monochromatic photons are fired at a lattice of atoms, the
scattered wave changes particularly in frequency as a function of the angle of reflection. In 1923, Arthur Compton ${ }^{6}$ demonstrated that x-rays (thus photons with little energy) are scattered by relatively free electrons (in remote shells) while losing their energy, in other words at a much lower frequency $v$ (Wissman 2004; Baur 1985, p. 78; Cottereau and Lefebvres 1971, p. 102; Shultis and Faw 2000,

[^51]
(the Marguet collection)

Fig. 3.11 Compton
scattering

p. 33; Filippi 1965, p. 220). Further, the difference in wavelength is given experimentally by the following law:

$$
\lambda_{\text {scattered }}-\lambda_{\text {incident }}=\lambda_{\text {Compton }}(1-\cos \theta)
$$

where $\theta$ is the angle of deviation of the photon. The constant $\lambda_{\text {Compton }}$ has been found to be the following for electrons:

$$
\lambda_{\text {Compton }}=\frac{h}{m_{e^{-}} c}=2.4262 \times 10^{-12} \mathrm{~m}
$$

The kinematics of collision may be considered as elastic scattering of the photon on a free electron. The conservation of energy and of the quantity of movement is given by:

$$
\left\{\begin{aligned}
h v & =h v^{\prime}+m_{e^{-}}(\gamma-1) \\
h v & =h v^{\prime} \cos \theta+m_{e^{-}} \sqrt{\left(\gamma^{2}-1\right)} \cos \varphi \quad \text { where: } \quad \gamma=1 / \sqrt{1-\frac{v^{2}}{c^{2}}} \\
0 & =h v^{\prime} \sin \theta+m_{e^{-}} \\
\left(\gamma^{2}-1\right) & \sin \varphi
\end{aligned}\right.
$$

The energy of the scattered photon is maximal at $\theta=0$. For a of $90^{\circ}$ right angle, the shift in wavelength is $0.024 \AA$. The physical explanation for this phenomenon involves the quantity of movement $p=h v / c=h / \lambda$ of a photon of zero mass at rest that undergoes collision with an electron (Fig. 3.11).

The conservation of kinetic energy $(E=p c$ before the collision, assuming that the electron is immobile, $E=p^{\prime} c+T_{e^{-}}$after the collision, assuming the electron to be nonrelativistic) and of the quantity of movement projected on the incident direction and its perpendicular direction, leads to the following relationships:

$$
\left\{\begin{array} { l } 
{ h v = h v ^ { \prime } + T _ { e ^ { - } } } \\
{ ( p _ { e ^ { - } } ) ^ { 2 } = T _ { e ^ { - } } ^ { 2 } + 2 m _ { e ^ { - } } c ^ { 2 } T _ { e ^ { - } } } \\
{ \vec { h v } } \\
{ \frac { h v ^ { \prime } } { c } = \frac { \vec { p _ { e ^ { - } } } } { c } }
\end{array} \left\{\begin{array}{l}
\frac{h}{\lambda}=\frac{h}{\lambda^{\prime}} \cos \theta+p_{e^{-}} \cos \varphi \\
\frac{h}{\lambda^{\prime}} \sin \theta=p_{e^{-}} \sin \varphi \\
\lambda^{\prime}-\lambda=\frac{h}{m_{e^{-}} c}(1-\cos \theta)
\end{array}\right.\right.
$$

The energy of the scattered photon decays according to the following formula:

$$
h v^{\prime}=\frac{h v}{1+(1-\cos \theta) \frac{h v}{m_{e}-c^{2}}}
$$

Since the energy of the scattered photon is never zero, the incident photon is never completely absorbed, unlike in the case of the photoelectric effect. Note that the shift in wavelength is independent of the incident wavelength and that this shift is greater for X photons than for visible light at a higher wavelength. Moreover, the approximation of the resting electron is more valid in the case of $x$ photons with a great amount of movement. The Compton effect thus corresponds to a photon yielding only part of its energy in expelling an electron. This is known as incoherent diffusion. Compton showed that electrons are always expelled forwards, while photons may undergo backscattering. The energy of an electron with Compton's effect is greater for a particle moving forward in relation to the incidence. Compton's effect is preponderant between 100 keV and 2 MeV . The probability of interaction (linear attenuation due to the Compton effect), which varies little with energy, is usually denoted $\sigma$ (Fig. 3.12).

Precise theoretical analysis of the angular deviation of the photon striking a free electron as a result of the Compton effect, and not involving an isotope, was conducted in 1928 in Copenhagen by Swedish physicist Oskar Klein (1894-1977) and Japanese physicist Yoshio Nishina (1890-1951). Using the quantum theory of electrodynamics, they established the formula for the differential cross section for scattering as a function of the solid angle (Mayo 1998, p. 292; Shultis and Faw 2000, p. 41):

$$
\begin{align*}
\text { Klein-Nishinaformula (1929) : } & \frac{d \sigma(E, \theta)}{d \Omega} \\
& =\frac{r_{e}^{2}}{2}\left[P(E, \cos \theta)-\sin ^{2} \theta P^{2}(E, \cos \theta)+P^{3}(E, \cos \theta)\right] \tag{3.3}
\end{align*}
$$

where $r_{e}=2.817 \times 10^{-13} \mathrm{~cm}$ and $P(E, \cos \theta)$ is the relation between the energy of the photon before and after collision:

$$
P(E, \cos \theta)=\frac{1}{1+\frac{E}{m_{e} c^{2}}(1-\cos \theta)}
$$



Fig. 3.12 Compton effect


Oskar Klein (left) and Yoshio Nishina (right) (Public domain)
The differential cross section as a function of the angle of deviation is given by:

$$
\frac{d \sigma(E, \theta)}{d \theta}=2 \pi \sin \theta \frac{d \sigma(E, \theta)}{d \Omega}
$$

The energy of the photon after collision is:

$$
E_{\otimes}=E \cdot P(E, \cos \theta)=E /\left[1+\frac{E}{m_{e} c^{2}}(1-\cos \theta)\right] .
$$

The higher the energy of the incident photon, the greater the probability of the photon being scattered forwards. From 1 MeV upwards, backscattering may be ignored. Note that the angular distribution of photons is not dependent on the type of matter traversed, because of the hypothesis of the free electron initially posited to create the Klein-Nishina formula. In the case of an electron bound to the electron cloud, a correction to the model is required. In 1975, Hubbell et al. proposed the following correction:

$$
\left.\frac{d \sigma(E, \theta)}{d \Omega}\right|_{\text {bound }}=\left.\frac{d \sigma(E, \theta)}{d \Omega}\right|_{\text {free }} . S\left(\frac{\sin (\theta / 2)}{\lambda}, Z\right)
$$

where the term $S([\sin (\theta / 2)] / \lambda, Z)$ depends both on the wavelength $\lambda_{\text {incident }}$ of the incident photon and on the chemical body (via the atomic number $Z$ ) to which the electron is bound. Quantitatively, factor $S$ is lower than one for forward-scattered photons and, more particularly, for low energy levels or high $Z$ numbers. In concrete terms, photons are more back-scattered at low energy. If scattering involves the strongly bound electron, the formula must take into consideration the mass of the nucleus and that of the electron, and the shift in wavelength becomes negligible. This is what happens with atoms having high $Z$ values and it is why the Compton effect is more readily observable for atoms with low $Z$ values.

The effective Compton cross section is obtained by integrating the KleinNishina formula for all angular directions. It has been shown (Baur 1985, p. 85) that this cross section tends towards zero as the energy of the incident photon tends towards infinity and that it tends towards the Thomson cross section $8 \pi r_{e}^{2} / 3$ as the incident energy tends towards zero.

### 3.3.6 Pair Production

When a photon of extremely high energy ( $>1 \mathrm{MeV}$ ) passes through an electromagnetic field (near the nucleus), it may disappear with an electron-positron pair being created (Kahan 1963, p. 57). This event can only occur in the vicinity of the nucleus since otherwise the impulse could not be conserved. Indeed, the impulse balance for a photon producing an electron-positron pair is written as follows (Fig. 3.13):

$$
\left\{\begin{array}{l}
\frac{h v}{c}=p_{e^{-}} \cos \theta+p_{e^{+}} \cos \varphi \\
p_{e^{-}} \sin \theta=p_{e^{+}} \sin \varphi
\end{array}\right.
$$

Fig. 3.13 Pair production


In the specific case in which the angle of emission between the electron and the positron forms a right angle $(\theta+\varphi=\pi / 2)$, we have:

$$
\left(\frac{h v}{c}\right)^{2}=\left(p_{e^{-}}\right)^{2}+\left(p_{e^{+}}\right)^{2}
$$

The total conservation of energy is written:

$$
h v=\sqrt{p_{e^{-}}^{2} c^{2}+m_{e^{-}} c^{4}}+\sqrt{p_{e^{+}}{ }^{2} c^{2}+m_{e^{+}}{ }^{2} c^{4}}
$$

Clearly, in the case of a right angle, these two expressions are incompatible, suggesting that such a process is impossible in isolation. In reality, the atomic nucleus near where the pair is produced contributes to the impulse balance through a recoil movement that participates in the impulse and energy balance. If we ignore the recoil energy, the energy balance equation is approximately correct.

Since the mass of the electron is $0.511 \mathrm{MeV} / \mathrm{c}^{2}$, as is the mass of the positron, pair production cannot occur unless the energy of the incident photon is above the threshold: $h v>1.022 \mathrm{MeV}$. This phenomenon becomes preponderant at high energies ( $>5 \mathrm{MeV}$ ). The energy balance is written:

$$
T_{e^{-}}+T_{e^{+}}=h v-2 m_{e^{-}} c^{2}
$$

The positron, antimatter of the electron, cannot survive very long in matter (Fig. 3.14).

As soon as it encounters an electron, both disappear and are transformed into photons, thus verifying the law of conservation of energy. Conservation of the impulse indicates that the two photons are emitted in opposite directions. The

Fig. 3.14 Pair production

probability of interaction (linear attenuation through pair production) is classically labelled $\pi$ and varies approximately in relation to $\rho Z^{2} / A$ (Cahen and Treille 1963). Bethe and Heitler showed that the effective cross section of pair production in the field of a nucleus increases rapidly with the energy of the photon once the threshold has been exceeded, and then tends towards a limit worth (Cottereau and Lefebvres 1971, p. 120):

$$
\sigma_{\text {pair }}=\alpha r_{0}^{2} Z^{2}\left[\frac{28}{9} \ln \left(183 Z^{-\frac{1}{3}}\right)-\frac{2}{27}\right] \text { for a photon of energy greater than }
$$

500 MeV
Where $\alpha=\frac{1}{4 \pi \varepsilon_{0}} \frac{e^{2}}{\hbar c}=\frac{1}{137}$ is the fine structure constant ${ }^{7}$ and $r_{0}=\frac{1}{4 \pi \varepsilon_{0}} \frac{e^{2}}{m_{e^{-}} c^{2}}=2.818$ fm is the classical electron radius.
Pair production can also occur more rarely in an electron field, although because of its small mass, it will remove extensive kinetic energy, giving a higher energy threshold of pair production, i.e. $4 m_{e^{-}} c^{2}=2.04 \mathrm{MeV}$ (GA Vol. 1, 1967, p. 88).

[^52]

The historic photo on the left (Public domain) and the US postal stamp containing the error issued in 2001 on the right (The Marguet collection).

Beyond 10 MeV , the screen effects of atomic electrons, particularly with heavy nuclei such as lead, tend to reduce the occurrence of pair production.

### 3.3.7 Cumulative Effects

(Valentin 1982a, b, p. 166)
If we plot the attenuation coefficients for each interaction, we see that the main effects are: a photoelectric effect at low energies, followed by the Compton effect, and finally the emergence of electron-positron pairs. Mass attenuation is the sum of these three effects:

$$
\frac{\mu}{\rho}=\frac{\tau}{\rho}+\frac{\sigma}{\rho}+\frac{\pi}{\rho}
$$

where $\tau / \rho$ is the mass attenuation due to the photoelectric effect, $\sigma / \rho$ is the mass attenuation due to the Compton effect, and $\pi / \rho$ is the mass attenuation due to the pair-production effect.
(Hine and Brownell 1956, p. 81) gives the corresponding curves for air and aluminum (p. 84). Mass attenuation is a function of the mass fraction of the components of a given medium:

$$
\frac{\bar{\mu}}{\bar{\rho}}=\sum_{i} \frac{m_{i}}{m_{\text {total }}}\left(\frac{\mu}{\rho}\right)_{i}
$$

Rayleigh-Thomson scattering is always negligible, except for low-energy photons. To each of these coefficients, we generally attribute the index $t$ for transferred or $d$ for diffused. For information, Figs. 3.15 and 3.16 provide the attenuation coefficient in $\mathrm{cm}^{-1}$ for lead (highly attenuating for photons) and water.

### 3.3.8 Scattered Radiation and Build-Up Factors

(Harrison 1958)
For argument, let us take an isotropic source $S_{[\gamma / s]}$ of $\gamma$ rays. The $\gamma$ flux (often called intensity) in a vacuum (i.e. without attenuation) is given by the standard formula of the inverse of the square root of distance:

$$
I_{\left[\gamma / \mathrm{cm}^{2} / \mathrm{s}\right]}=\frac{S_{[\gamma / \mathrm{s}]}}{4 \pi r_{[\mathrm{cm}]}^{2}}
$$

Fig. 3.15 Attenuation coefficients for photons in lead


Fig. 3.16 Attenuation coefficients for photons in water


If this source is placed in an attenuating medium, the previous formula requires correction:

- Exponential attenuation in a straight line of the fine beam of $\gamma$ rays: $e^{-\mu r}$. For beams passing through several thicknesses $x_{i}$ of different attenuation materials $\mu_{i}$, the correction is written $\exp \left(-\sum_{i} \mu_{i} x_{i}\right)$.
- Scattered radiation (for a broader beam) which increases the intensity of the measuring point via the coefficient known as the accumulation factor or more commonly build-up factor: $B u_{[-]}$(Lamarsh and Baratta 2001, p. 551; Métivier 2006, p. 281; Price et al. 1957, p. 40).

The intensity is written as: $I_{\left[\gamma / \mathrm{cm}^{2} / \mathrm{s}\right]}=\frac{S_{[\gamma / \mathrm{s}]}}{4 \pi r_{[\mathrm{cm}]}} B u e^{-\mu r}$
The accumulation factor may thus be defined as the ratio between the total intensity and the intensity of the radiation not deviated during its trajectory. The value of the accumulation factor depends on the nature and thickness of the matter being crossed, as well as the angle of incidence of the radiation, but also on the geometry and position of the sources. A build-up factor may also be defined by type of application, i.e. the deposited energy or dose. Precise calculation of build-up factors is generally complex and frequently involves reference calculations based on the Monte-Carlo method. In the 1950s, J.J. Taylor then J.R.A. Lakey proposed a practical though approximate analytical expression for the coefficient of the buildup factor (see Rockwell 1956, pp. 9 and 415 for the value of the coefficients for water, lead and concrete). Their approach involved expressing the build-up factor in the form of exponentials (the Taylor formula, not to be confused with the extremely well-known homonymic limited expansion):

$$
B u=A e^{-\alpha_{1} \mu x}+(1-A) e^{-\alpha_{2} \mu x}
$$

where $A, \alpha_{1}$ and $\alpha_{2}$ are constants that depend on the type of material crossed and the energy of the $\gamma$ rays. This expression allows the exponentials to be grouped together in the calculation of intensity and provides a formulation similar to that for the intensity of non-deviated rays, thus simplifying analytical calculations for simple geometries:

$$
I=\frac{S}{4 \pi r^{2}}\left(A e^{-\left(1+\alpha_{1}\right) \mu x}+(1-A) e^{-\left(1+\alpha_{2}\right) \mu x}\right)
$$

Taylor and Lakey have provided tabulated values for the coefficients $A, \alpha_{1}$ and $\alpha_{2}$ for the majority of materials used in radioprotection. ${ }^{8}$ Many authors have proposed more or less empirical formulae, based for example on the atomic

[^53]number. ${ }^{9}$ A more recent method ${ }^{10}$ offers an approximation of the accumulation factors for a multilayer problem) using recurrent reasoning based on two layers. The accumulation factor of a two-layer screen, in which the first layer is of thickness $x_{1}$ (in relation to the incident beam) and that of the second layer is $x_{2}$ (expressed as mean free path), is modelled as follows:
$$
B u\left(x_{1} \mid x_{2}\right)=\frac{B u_{1}\left(x_{1}\right)}{B u_{2}\left(x_{2}\right)} B u_{2}\left(x_{1}+x_{2}\right) F\left(x_{1}, x_{2}\right)
$$
where $F\left(x_{1}, x_{2}\right)$ is an adjustment function of the form $\left(\left(\alpha\left(x_{1}\right)+x_{2}^{\beta\left(x_{1}\right)}\right) / \alpha\left(x_{1}\right)\right)^{p}$ in which $\beta\left(x_{1}\right)>0$ and $p=-1,0$ or 1 as a function of the energy source and screen type. This formula is obviously empirical. The coefficients have been carefully calculated for different types of two-layer screen and for several energy sources, e.g. for a "steel-water" screen and also for a "water-steel" screen (the results are not the same, and the formula is not commutative since the order of the screens has real physical significance). By recurrence for the layers, we obtain the following accumulation factor for a screen comprising $n$ layers:
$$
B u\left(x_{1}\left|x_{2}\right| \cdots x_{n-1} \mid x_{n}\right)=\frac{B u\left(x_{1}\left|x_{2}\right| \cdots x_{n-2} \mid x_{n-1}\right)}{B u_{n}\left(\sum_{i=1}^{n-1} x_{n-1}\right)} B u_{n}\left(\sum_{i=1}^{n} x_{n}\right) F\left(x_{n-1}, x_{n}\right)
$$

The build-up factors for two layers have been provided for penetration levels of up to 30 mean free paths ( $m f p$ ) and qualification by comparing against the reference calculations show that the resulting error does not exceed $25 \%$ for extremely deep penetrations, which is completely acceptable in the radioprotection field.

### 3.3.9 Application of Photon Attenuation in Matter

We have seen that at the start of the twentieth century, x-rays were used in the medical field with great success. Another application of $\gamma$ radiation very widely used in the nuclear domain is non-destructive control testing (Lévêque et al. 1962, p. 85). Depending on the depths to be penetrated, photons of different energies are used to investigate the structure to be analyzed, and a film, placed on the other side of the structure, is exposed and contains the residual photons not absorbed during

[^54]
t , tube «Coolidge ${ }_{»} ; \mathrm{c}$, cathode; b , anticathode; T , transformateur du courant à haute tension; SS, connexions $+e t$ du courant à haute tension; GG, connexions $+e t-d u$ courant à basse tension alimentant le transformateur T; A, V, R, ampèremètre, voltmètre, rhéostat de réglage du courant à basse tension; M, milliampèremètre du courant à haute tension; $\mathbf{a}^{1}, \mathbf{u}^{1}, \mathbf{r}$, ampèremètre, voltmètre et rhéostat de réglage du courant d'alimentation de la cathode $\mathbf{~ B}$, batteric d'accumulateurs fournissant le courant à la cathode.

Fig. 3.17 The electrical apparatus used to produce photons (x-rays) from a Coolidge tube in order to investigate unrevealed cracks inside a piston, as seen in "La Science et la Vie" n${ }^{\circ} 30$, December 1916 (!) (Public domain, The Marguet collection)
passage through the medium. Consequently, all defects or cavities appear to be more marked on the film since more photons survive to strike the film in the preferential directions of travel through cavities, with photons being absorbed primarily by heavy materials (lead, uranium, etc.). The principle is completely identical to that of radiography in humans, although more energetic photons are used in order to penetrate heavy structures (Figs. 3.17 and 3.18).

Qualification of the procedures and setting of the exposure times may be carried out by use of reference photon transfer calculation codes [TRIPOLI (CEA), MCNP (Los Alamos), MODERATO (EDF), etc.]. By way of illustration, ${ }^{11}$ Fig. 3.19 presents a numeric simulation (MODERATO code using the Monte-Carlo method) of the firing of 10 million photons through a dummy piece of steel containing cylindrical holes of varying widths and heights (shown in grey in the figure). The structure of lines represents the outside contours of the test piece which is in the

[^55]Fig. 3.18 The radiogram obtained with the previous apparatus, cracks and blowholes appear close to north-side, as seen in " $L a$ Science et la Vie" n ${ }^{\circ} 30$, December 1916. (Public domain, The Marguet collection)


PHOTOGRAPHIE DU FOND DU PISTON
On y distingue les criques et soufflures révélées par les rayons $\mathbf{X}$.

Fig. 3.19 Digital firing of photons, using the MonteCarlo method, into a test piece containing cylindrical holes of various sizes: the trajectories of photons irradiating the item from above are shown. Some undergo scattering inside the piece. Below the test piece, we see the film imprinted by photons emerging via the lower surface and shown in Fig. 3.20 (Courtesy Schumm 2008)

Fig. 3.20 Digital film simulating direct photon flux without collision: the larger the empty cylinders, the greater the imprint on the film. Note that the film is completely imprinted outside the base of the item since there is no attenuation in this region

shape of a cylindrical segment. The trajectories are shown of the photons "raining down" on the upper surface of the test piece and in some cases undergoing scattering inside the piece. The trajectories of undeviated photons are occasionally referred to as ballistic trajectories, in contrast with scattered trajectories.

Photons crossing the test piece in a straight line without undergoing scattering imprint the film as shown in Fig. 3.20. Those scattering due to multiple collisions may nevertheless reach the film, as may be seen in Fig. 3.21. It is clear that scattering radiation in itself is difficult to exploit. Consequently, most analytical methods use only direct (so-called "ballistic") radiation. The actual image obtained by the person conducting the test would in fact be a superimposition of the images in Figs. 3.20 and 3.21. The Monte-Carlo method simulates the individual behavior of each photon by random selection of possible interactions. The law of large numbers provides a satisfactory probability for the result being sought by simulating a very great number of particles. With 10 million photons, the image is

Fig. 3.21 Digital film simulating scattered photon flux reaching the film (at least one collision): here the geometry is practically no longer discernible. This diffuse radiation blurs the actual image, which is in reality a superimposition of the present image and the image of Fig. 3.20

sufficiently clear to be usable. This radiography technique for analysis of items to be tested is used for the nondestructive detection of defects. Note that identical techniques exist with neutrons, which are stopped by chemical bodies with lower mass numbers, in contrast with photons. Moreover, the diffusion of neutrons in crystals has led to important theoretical developments (Krivoglaz 1969; Krawitz 2001, p. 105). This technique thus complements radiography and is used for example to detect illicit substances in containers transported by sea. The two techniques, using neutrons and photons, may ultimately be used in complementary fashion to cover all elements in the periodic table. Nguyen and Truong (2006) proposes a wide range of applications for scattering gamma radiation in the field of imaging. Herman (1980) provides a detailed presentation of the principle of tomography, which uses ballistic gamma radiation coupled with relevant specific deconvolution signal-processing (e.g. Radon transformation) (Jansson 1984).

### 3.3.10 Photoneutrons

(Annual Review of Nuclear Science, Vol. 2 1953, p. 105; Cameron 1982, p. 36; Goldstein 1959, p. 55)

With sufficiently high-energy photons, neutron production is observed on light nuclei ${ }^{12}$ (Keepin 1965, p. 142), and we should bear in mind the photoneutron reaction for beryllium (Keepin 1965, p. 147), the high yield of which led to hopes at the start of the nuclear age that a fission reaction might be maintained using massive quantities of beryllium, but which proved impossible (Bekurts and Wirtz 1964, p. 31):

[^56]${ }_{4}^{9} B e+\gamma \quad \rightarrow \quad{ }_{4}^{8} B e+{ }_{0}^{1} n \quad$ threshold of 1.67 MeV , neutron at 25 keV
Beryllium also produces neutrons when irradiated with $\alpha$ particles. In addition, a photo-neutron reaction occurs on deuterium in water, but at a higher threshold:
$$
{ }_{1}^{2} H+\gamma \quad \rightarrow \quad{ }_{1}^{1} H+{ }_{0}^{1} n \quad \text { threshold of } 2.21 \mathrm{MeV}
$$

Naturally, this reaction occurs mainly in heavy water reactors. In power reactors, the photon source is dependent in part on the occurrence of $(n, \gamma)$ reactions and on the decay of fission products (during operation but also at close-down, which accounts for the source of neutrons even in reactors that have been closed down for long periods). In industrial settings, rod assemblies containing antimony-beryllium pellets are used as neutron sources to start up reactor cores that have already been irradiated. Neutron activation of ${ }_{51}^{124} \mathrm{Sb}$ produces extremely high-energy photons at 1.857 MeV that activate the beryllium, producing around 1 million neutrons per 1 Curie of decay (GA, Vol. 1, 1967, p. 99).

$$
\begin{aligned}
{ }_{0}^{1} n+{ }_{51}^{123} \mathrm{Sb} \rightarrow & { }_{51}^{124} \mathrm{Sb} \stackrel{\beta^{-}}{\underset{50.2}{6} \text { days }}{ }_{52}^{124} \mathrm{Te}+{ }_{-1}^{0} e^{-} \\
& +\quad \gamma(1.857 \mathrm{MeV})
\end{aligned}
$$

### 3.3.11 Photofission

The phenomenon of fission induced by photon absorption is generally ignored in reactors, despite the fact that it is not completely absent. This special kind of fission is always a threshold reaction (around 5 MeV , see Table 3.2), the effective cross section of which presents a shape roughly similar to a peak at around 15 MeV (Fig. 3.22). With higher energy photons (GeV), photofission becomes more preponderant, but such energy levels are not encountered in power reactors.

### 3.4 Measuring Radiation

(Duquesne et al. 1960; Lilley 2001, p. 152; Lévêque et al. 1962, p. 22; Sharpe 1964)
Photons are generally measured using an instrument known as a photomultiplier, which works by transforming incident photon radiation into electrons that are then counted using a classical electron chain (Samueli et al. 1968, p. 23). The photons

Table 3.2 Photofission reaction thresholds for some fissile isotopes

|  | ${ }_{92}^{233} U$ | ${ }_{92}^{235} U$ | ${ }_{92}^{238} U$ | ${ }_{90}^{232} \mathrm{Th}$ | ${ }_{94}^{239} \mathrm{Pu}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Photofission threshold $[\mathrm{MeV}]$ | 5.18 | 5.31 | 5.08 | 5.40 | 5.31 |



Fig. 3.22 General shape of the cross-section for photofission of fissile isotopes


Fig. 3.23 Internal schema of a photomultiplier
interact with the cathode of the photomultiplier and detach electrons according to the principle of the photoelectric effect. These electrons are collimated in a multiplication chamber, where they interact with dynodes so as to amplify the beam, and they are then sent to the anode, from which they are evacuated by the system connected to the instrumentation (Fig. 3.23). The photomultiplier produces an exitslit charge proportional to the number of incident photons reaching the photocathode. If $N$ is the number of photoelectrons emitted by the cathode, the photomultiplier measures the quantity $G N$ electrons reaching the anode. Factor $G$ is the gain of the photomultiplier, which depends on the number of internal dynodes. If the photomultiplier is subjected to packets of photons or pulses sufficiently far apart in time, it reacts as though these events were separate. Following amplification, the height of the pulse in question may be measured. Because of the statistical variations inherent to the phenomenon of conversion of photons to electrons, as well as the multiplication of the electrons by the dynodes, the charge of the outgoing signal may vary for a single pulse of incident photons. The Gaussian
distribution of the outgoing signal thus restricts the resolution of the device, and in particular, the energy resolution of the scintillation method (Samueli et al. 1968, p. 5). The photomultiplier is an essential instrument for the scintillation technique and for Cherenkov counting (Progress in Nuclear Physics, Vol 8, 1960, p. 195; Instrumentation en physique nucléaire (Instrumentation in Nuclear Physics) 1989, p. 249). The scintillation counter is a radiation counter comprising three main components: a scintillating medium that produces light under the effect of ionizing radiation, one or more photomultipliers that transform the light (photons) into electrical impulses, and an acquisition chain that transforms this current into a usable signal.

Cherenkov counting involves a medium in which light is created via the Cherenkov effect from the electromagnetic radiation to be measured, as well as one or more photomultipliers optically coupled with the Cherenkov medium, and naturally, an acquisition chain.

If the source to be measured is too intense, the photomultiplier response will no longer be linear and the outgoing signal is saturated. Care must therefore be taken to use the photomultiplier within its linear range.

### 3.5 Interaction of Electrons with Matter

(Cauchois and Héno 1964; Miley 1970, p. 90)
Electrons have been intensively studied as fundamental vectors of electricity in the form of free electrons, in other words not electrons gravitating around the nucleus. The first famous experiment on the interaction between electrons and matter was conducted in 1891 in a Crookes tube in which "cathode" rays, as they were then called because they were emitted by a negatively charged cathode, produced a strange green fluorescence on the bottom of the glass tube. At the start of the twentieth century, exponential attenuation was observed along the travel of $\beta^{-}$particles in matter for which it was possible to measure mass attenuation in the same way as for photons (Fournier and Guillot 1933). The passage of electrons through matter, which was precisely modelled using a transport equation very similar to that for neutrons, produces different interactions such as:

- elastic scattering on the nucleus of target atoms (Coulomb diffusion), resulting in a slight loss of energy. The probabilities of interaction (effective cross sections) are given in the classic form of Spencer's tables. ${ }^{13}$ Electrons, being light particles, are deviated far more frequently than heavier $\alpha$ particles. Total statistical deviation is considered (Cahen and Treille 1963) proportional to the ratio between the square root of the distance travelled and the energy of the particle;

[^57]- inelastic scattering on the electrons of the atom. This form of scattering is the main phenomenon responsible for energy loss at several MeV . It involves excitation of peripheral electrons followed by de-excitation via the emission of x-rays. The theory of Möller (1932) produces effective cross sections (Mayo 1998, p. 276), with modelling of this phenomenon for use in Hans Bethe's general theory of approximation of continuous slowing down, which we shall discuss later;
- inelastic diffusion on the nucleus is a phenomenon that occurs below the level of several MeV . It results in the production of Bremsstrahlung photons, clearly modelled in the theory of Bethe and Heitler (Cottereau and Lefebvres 1971, p. 118), which gives the differential cross-section for production of a braking photon in the frequency range $[v, v+d v]$ :

$$
\sigma(v)=4 \alpha r_{0}^{2} Z\left(Z+\xi_{Z}\right) \log \left(183 Z^{-\frac{1}{3}}+\frac{1}{8}\right) \frac{d v}{v}
$$

where $\alpha=\frac{1}{4 \pi \varepsilon_{0}} \frac{e^{2}}{\hbar c}=\frac{1}{137}$ is the fine structure constant and $r_{0}=\frac{1}{4 \pi \varepsilon_{0}} \frac{e^{2}}{m_{e}-c^{2}}=2.818 \mathrm{fm}$ is the classic electron radius. $\xi_{Z}$ is a coefficient that depends to a small degree on $Z$, i.e. 1.4. for hydrogen and 1.14 for uranium. A constant value of 1.3. may be used.

- the production of secondary photons (by Bremsstrahlung or fluorescence photons). These photons may themselves produce electrons by means of the photoelectric effect, the Compton effect or pair production, hence the concept of the photoelectric cascade.

At high energies, electron/photon coupling is very strong, but the phenomenon has a great tendency to occur in a forward direction (it is anisotropic), enabling certain simplifications in the calculation of angular distributions. Bethe's theory of continuous slowing down (Continuous Slowing-Down Approximation or CSDA) models the interactions of electrons, which are innumerable, by means of a continuous phenomenon via the concept of stopping power (Hine and Brownell 1956, p. 27), in other words, the mean energy loss across the distance of the trajectory $-d E / d x$, which is also known in biological applications as linear energy transfer (LET) [a name ascribable to Zirkle (Goldstein 1959, p. 21)]. Since certain electrons lose more than the mean, the studies undertaken by Landau, O. Blunck and K . Westphal ${ }^{14}$ led to distribution of energy loss that includes the broadening due to loss of energy resulting from collision and radiation. The electron transport equation is written in linear form:

[^58]\[

$$
\begin{aligned}
& \frac{1}{v} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, E, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, E, t)+\Sigma_{t}(E) \Phi(\vec{r}, \vec{\Omega}, E, t) \\
& \quad=\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} \Sigma_{s}\left(E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \overrightarrow{\Omega^{\prime}}, E^{\prime}, t\right) d \vec{\Omega}^{\prime}
\end{aligned}
$$
\]

where:
$\Phi(\vec{r}, \vec{\Omega}, E, t)$ is the flux of electrons of energy $E$ at point $\vec{r}$ in direction $\vec{\Omega}$ and at time $t$,
$\Sigma_{t}(E)$ is the probability (macroscopic cross-section) of interaction per unit of path travelled
$\Sigma_{s}\left(E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right)$ is the probability per unit of path travelled of scattering towards energy $E$ and direction $\vec{\Omega}$

This integro-differential Boltzmann equation expresses the balance of particles between their appearance and disappearance. We seek to express the cumulative effect of interactions throughout a given trajectory by expressing the temporal derivative as a function of a derivative to the path $\ell$ :

$$
\frac{1}{v} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, E, t)}{\partial t}=\frac{\partial \Phi(\vec{r}, \vec{\Omega}, E, t)}{\partial \ell}
$$

where the path followed is: $\ell=\int_{0}^{t} v\left(t^{\prime}\right) d t^{\prime}$
The notion of stopping power $\frac{d E}{d \ell}(\ell)$ is inserted in the calculation for energy loss:

$$
E_{0}-E(\ell)=\int_{0}^{\ell} \frac{d E}{d \ell}\left(\ell^{\prime}\right) d \ell^{\prime}
$$

### 3.5.1 Ionization

(Boutry 1962, p. 312)
Ionization indicates the stripping off of a planetary electron by a moving electron (Kahan 1963, p. 51). The corresponding atom is thus no longer neutral but is positively charged since it has lost an electron and is called an ion. A mean energy of 35 eV is required in gases such as xenon to produce ionization. During the interaction, the incident electron loses energy corresponding to the binding energy of the planetary electron as well as the kinetic energy transferred to it.

The phenomenon of ionization is especially important as the charge and mass of the incident particle increase. Several electrons on a single atom may be stripped off. Since the stripped electrons have speed, they are able in turn to ionize other

Fig. 3.24 Ionization

atoms in a cascade phenomenon that gradually decreases in step with the dissipation of energy of the emitted particles (Fig. 3.24).

In the 1920s, very many scientists studied ionization, particularly of gases and vapors. The reference (Bloch 1925; Herzberg 1991, p. 200) provides a table, already extremely precise for the time (1937), of the ionization potentials for many elements. The principle of ionization underlies a measuring device that played a key role in the history of particle physics: the Wilson chamber or cloud chamber.

### 3.5.2 Wilson Chamber

(Blanc 1966, p. 117)
The principle of the cloud chamber or Wilson chamber, named after its brilliant inventor, Scottish physicist Charles Thomson Rees Wilson (1869-1959), winner of the Nobel Prize in Physics in 1927, consists in visualizing the trajectory of a charged (ionizing) particle in a cloud of water steam (Born 1971, p. 40; Kahan 1963, p. 23). An ionizing particle, such as an electron, ionizes the atoms contained in a cloud formed of a gas saturated with water (or alcohol). If, at the same time, depressurization occurs inside the apparatus by increasing the volume of the chamber, both the pressure and the temperature decrease (Photo 3.3).

Thus, if the increase in volume is low, a balance is maintained between water and vapor: there is no massive condensation of vapor if the system is well calibrated, but the conditions remain at the extreme limit of condensation. Indeed, just as raindrops or snowdrops begin to aggregate by condensation around a "germ" (for example a minute dust particle), ions ionized by the passage of the electron cause visible condensation on a photograph that is sufficiently illuminated, enabling the trajectory of the particle to be visualized (Fig. 3.25).


Photo 3.3 Charles Wilson (1869-1957), winner of the 1927 Nobel Prize for physics (Public domain)


Fig. 3.25 Principle of the Wilson chamber used to visualize ionizing particles
His prodigious efforts in photographing more than 20,000 images in his Wilson chamber in 1925 enabled Patrick M. Blackett ${ }^{15}$ to identify a mere eight collisions, but these demonstrated the first transmutation of an atom of nitrogen 14 into oxygen 17 through the capture of an $\alpha$ particle.

[^59]$$
{ }_{2}^{4} \mathrm{He}+{ }_{7}^{14} \mathrm{~N} \rightarrow{ }_{8}^{17} \mathrm{O}+{ }_{1}^{1} \mathrm{H}^{+}
$$

Along with Guiseppe P. S. Occhialini, Blackett also provided experimental confirmation on February 7, 1933, of the existence of the positron, which had been discovered by Carl D. Anderson in 1932 among cosmic rays (Auger 1948; Capdevielle 1984).

### 3.5.3 Excitation

(Boutry 1962, p. 312)
The phenomenon of excitation was discussed earlier in relation to the production of x-rays. An incident electron excites a planetary electron and makes it change orbital; this is followed by reorganization of the electrons associated with the emission of an $X$ photon at low energy (100-10,000 eV) (Fig. 3.26).

### 3.5.4 Braking Radiation or Bremsstrahlung

An electron that has been slowed down by an electromagnetic field loses energy and emits a photon. At low energies, an x-ray photon is emitted during the course of deviation of the electron in the same way as a catapult releases a stone (the photon) when the rotating arm is blocked. This phenomenon of deceleration radiation is historically designated by the German term Bremsstrahlung (Kahan 1963, p. 48). It was discovered by Nikola Tesla (1856-1943), the Serbian genius of physics and engineering, whose name has been given to the official unit of magnetic fields (Fig. 3.27).


Fig. 3.26 Electron excitation

Fig. 3.27 Braking radiation or Bremsstrahlung


Electron at energy $E^{\prime}<E$

Fig. 3.28 Annihilation of electron/positron pairs

Photon


### 3.5.5 Annihilation

When an electron encounters its antiparticle, the positron, the two are mutually annihilated and two energetic photons are created. Positrons are slowed down in matter in more or less the same way as electrons. Annihilation is a phenomenon that always occurs between a particle and its antiparticle (Fig. 3.28).

### 3.6 Cherenkov-Mallet Effect

If a charged particle of low mass and high energy (e.g. an electron) is emitted at a speed greater than that of light $c / n$ in a medium with a refractive index $n$ (NB: not the speed of light in a vacuum, which is a physical limit that cannot be exceeded) (Born 1971, p. 42; Berthelot 1956, p. 58; Cauchois and Héno 1964, p. 23 and p. 74), the particle interacts with the refractive medium through which it crosses and disturbs the electron shells of the nuclei in the vicinity of its trajectory. The electrons are deviated from their initial position before returning to their previous orbit. We speak of polarization of the medium. Small dipoles appear along the entire trajectory of the charged particle (10 billion times per meter in water), and of a field of dissymmetric polarization and emission of a cone of electromagnetic
radiation during passage through a polarizable medium (such as water). In transparent media such as water, air, or glass, depolarization occurs through the emission of a light wave at all wavelengths, but predominantly in the blue and ultraviolet. This radiation, caused by the depolarization of the medium, may occur in the domain of visible light waves to form a shock wave identical in principle to the sound waves generated when a supersonic aircraft breaks the sound barrier. This is the Cherenkov-Mallet effect. ${ }^{16}$ This phenomenon of bluish luminescence in water caused by radioactive products was detected in the 1900s by Marie Curie, and then analyzed in greater detail by Lucien Mallet (Fig. 3.29).

Although initially associated with the fluorescence of solutes in water (discrete de-excitation rays), the luminous spectrum was shown in 1926 by French physicist Lucien Mallet to be continuous, contrary to what was obtained in the case of fluorescence. Cherenkov showed as of 1934 that this continuous radiation was independent of the composition of the medium through which it passed. Where the speed of the charged particle is low, depolarization is incoherent. Since the waves emitted by the atoms are superimposed on one another in a disordered fashion and they are never in phase. However, where the speed of the charged article is very high, emission by each atom encountered causes a coherent wave front emitted in the blue and ultraviolet wavelengths and visible in the case of water [for an electron at an energy of at least 0.26 MeV (Cahen and Treille 1963)], which

[^60]

Two stamps celebrating the Russian physicist, Pavel Cherenkov (The Marguet collection).

Fig. 3.29 The CherenkovMallet effect

follows the particle as a cone of light. The cone of light is thus blue "at the surface" of the cone and dark inside the cone. It is the multiple trajectories, followed by electrons, that create luminosity visible everywhere. Ultimately, this is equivalent to the classic Compton effect in which the relativistic Compton recoil electron is produced by "hard" photons arising from fission products (GA Vol. 1 1967, p. 78). Depolarization of the medium (in this case, water) under the effect of $\beta^{-}$radioactivity leads to the emission of photons in the visible spectrum. This is the case of pools containing radioactive materials (fuel). Within the visible domain, a bluish light is emitted. Where $n$ is the refractive index of the refractory medium, if $c>v>c / n$, the cosine of angle $\alpha$ of the collision cone is given by:

(The Marguet collection) Plaque from the Paris Mint

$$
\sin \alpha=\cos \theta=\frac{c}{v n}
$$

We are more interested in angle $\theta$ beneath which a motionless observer sees the light wave moving towards him. For a maximum speed of $v=c$, the maximum angle attainable in air ( $n=1.0003$ ) is $1.4^{\circ}$, compared with $41^{\circ}$ in water $(n=1.33)$. The energy threshold of the Cherenkov effect is given by:
$E_{\text {threshold }}=\left(\sqrt{1+\frac{1}{n^{2}-1}}-1\right) m c^{2}$, or 0.265 MeV for electrons in water.
The Cherenkov-Mallet effect enables the ready identification of irradiated fuels in a deactivation pool, with the electrons emanating from the $\beta^{-}$radiation of the fission products. The Cherenkov-Mallet effect is also used to detect the trajectories of muons produced by the interaction between neutrinos and the Earth. This is the underlying principle of the Antarès submarine detector, installed at a depth of 2400 m off the island of Porquerolles (South of France) and of which the photomultipliers, arranged in $3 D$ array at intervals of around 10 m and oriented towards the depths, measure the light of the ascending muons produced by the interaction of neutrinos arriving after travelling from the opposite side of the Earth. Electronic neutrinos are produced primarily by the combustion of our Sun at a rate of $65 \times 10^{9}$ neutrinos per second and per $\mathrm{cm}^{2}$. It is known that extremely high energy neutrinos ( $>100 \mathrm{GeV}$ ) produce muons that are collinear since they are expelled forwards.

### 3.7 Charged Particles: Rutherford Diffusion

(Cauchois and Héno 1964; Cottereau and Lefebvres 1971, p. 9; Delcroix 1959, p. 8; Mahan et al. 1970, p. 402; Mayo 1998, p. 263; Valentin 1982a, b, p. 9)

The charged particles are submitted to an electromagnetic field. As they evolve in matter, the charged particles transfer energy to electrons in the electron cloud of the atoms making up the medium through which they pass. The atom may then become either excited if the electron receiving the energy remains in the electron cloud, or ionized if the electron is ejected by the passage of the particle. For a charged particle, interaction with the electrons of the atom is more likely than interaction with the atomic nucleus, since on one hand the nuclear forces involved act over a very short range, as was seen earlier, and on the other, if the particle is positively charged, as is the case with $\alpha$ particles, it will be repelled by the protons in the nucleus. Rutherford analyzed the deviation of an $\alpha$ particle by an atomic nucleus. The equations are those for Coulomb attraction between two positive charges (Berthelot 1956, p. 18). When a charged particle of mass $m$ and charge $z$ arrives in the electromagnetic field of the target of mass $M$ and charge $Z$, creating a central force field of potential $V(r)=z e Z e /\left(4 \pi \varepsilon_{0} r\right)$, it undergoes a deflection that may be calculated using the laws of mechanics and electromagnetics (Bayet 1960, p. 57). If we disregard the relativistic effects and we assume the target to be immobile, the conservation of kinetic energy and of change in potential energy


Fig. 3.30 Deflection of a charged particle in a central potential field
may be transposed as follows, using the notations in Fig. 3.30, (Sigmund 2008, p. 75; Jouguet 1964, p. 17):

$$
E_{c}=\frac{1}{2} m\left(\left(\frac{d r}{d t}\right)^{2}+r^{2}\left(\frac{d \varphi}{d t}\right)^{2}\right)+V(r)=\frac{1}{2} m v_{-\infty}^{2}
$$

The speed varies according to the curvilinear coordinate $s$ and assumes the value $v\left(s_{l}\right)$ at the point nearest the target located at distance $l$. Distance $b$ is classically called the impact parameter (Foderaro 1971, p. 46; Sigmund 2008, p. 41, note p; Delcroix 1959, p. 14). This is the closest distance at which an undeviated neutral particle passes. Inside a central force potential, the trajectory of the incident particle forms a hyperbola, the focus of which is the central target, and $\theta$ is the scattering angle of the particle. Conservation of the kinetic moment $L$ (Sigmund 2008, p. 74) of the target + particle together is written as follows, for a fixed target:

$$
m v_{(-\infty)} b=m v_{\left(s_{l}\right)} l \quad \text { hence } \quad v_{\left(s_{l}\right)}^{2}=v_{-\infty}^{2} \frac{b^{2}}{l^{2}}
$$

Conservation of kinetic energy using these definitions of variables is written as follows (Fig. 3.31):

$$
\frac{1}{2} m v_{-\infty}^{2}=\frac{1}{2} m v_{\left(s_{l}\right)}^{2}+\frac{z Z e^{2}}{4 \pi \varepsilon_{0} l}
$$

Inserting this in the energy equation gives: $m v_{-\infty}^{2} l^{2}=m v_{-\infty}^{2} b^{2}+\frac{z Z e^{2}}{2 \pi \varepsilon_{0}} l$
Because of the properties of the hyperbola, assuming $a^{2}+b^{2}=c^{2}$, we have $l=c+a$, and thus: $v_{-\infty}^{2}(c+a)^{2}=v_{-\infty}^{2}\left(c^{2}-a^{2}\right)+\frac{z Z e^{2}}{2 m \pi \varepsilon_{0}}(c+a)$

Namely: $a=\frac{z Z e^{2}}{4 m \pi \varepsilon_{0} v_{-\infty}^{2}}$ and $\tan \frac{\theta}{2}=\frac{a}{b}=\frac{z Z e^{2}}{4 m \pi \varepsilon_{0} v_{-\infty}^{2} b}$
If we fire a given number of particles $n_{0}$ per unit of area and per second, the number of particles having an impact parameter $b$ up to $d b$ is $n_{0} 2 \pi b d b$ due to symmetry of revolution. The probability of a particle being scattered at angle $\theta$ is given by:


Fig. 3.31 Electrostatic deviation of a charged particle in an electromagnetic field

$$
\frac{d \sigma}{d \Omega}=\frac{2 \pi b d b}{2 \pi \sin \theta d \theta}
$$

Since: $d b=\frac{d\left(\frac{z Z e^{2}}{4 m \pi \varepsilon_{0} 0^{2} e^{\tan (\theta / 2)}}\right)}{d \theta}=\frac{1}{2} \frac{z Z e^{2}}{4 m \pi \varepsilon_{0} v_{-\infty}^{2} \sin ^{2}(\theta / 2)} d \theta$ we have:

Rutherford differential cross section : $\quad \frac{d \sigma}{d \Omega}=\frac{z^{2} Z^{2} e^{4}}{64 m^{2} \pi^{2} \varepsilon_{0}^{2} v_{-\infty}^{4} \sin ^{4}(\theta / 2)}$
This is the expression for the differential diffusion cross-section (Sigmund 2008, p. 78; Valentin 1982a, b, p. 14; Shultis and Faw 2000, p. 63) that enabled Rutherford to interpret his famous experiment on the scattering of $\alpha$ particles on gold foil.

The case of backscattering (Fig. 3.32) by a target $C$ at charge $Z$ is identical to the foregoing case, with the following notations:

$$
\theta+2 \varphi=\pi \quad \overline{A C}=\overline{A 0}+\overline{O C}=a+c \equiv l \quad \overline{K C}=2 a=2 c \cos \varphi \quad b=c \sin \varphi
$$

Giving:

$$
l=\frac{b(1+\cos \varphi)}{\sin \varphi}
$$

As before, the conservation of energy (for a fixed target) is always written:

$$
\frac{1}{2} m v_{-\infty}^{2}=\frac{1}{2} m v_{\left(s_{l}\right)}^{2}+\frac{z Z e^{2}}{4 \pi \varepsilon_{0} l}
$$

and conservation of the kinetic moment is: $m v_{(-\infty)} b=m v_{\left(s_{l} l\right.} l$
These equations are naturally completely identical in the event of forward scattering. These two qualities allow elimination of speed at the nearest point $v_{\left(s_{l}\right)}$, giving:


Fig. 3.32 Backscattering of a charged particle

$$
\begin{equation*}
b=\frac{z Z e^{2}}{4 \pi \varepsilon_{0} m v_{(-\infty)}^{2}} \tan \varphi=\frac{z Z e^{2}}{4 \pi \varepsilon_{0} m v_{(-\infty)}^{2}} \operatorname{cotan} \frac{\theta}{2} \tag{3.5}
\end{equation*}
$$

Let us now examine a thin target of thickness $\Delta x$ in centimeters (if the target is too thick, no $\alpha$ particles will be scattered since they will all be absorbed) and of area $1 \mathrm{~cm}^{2}$. This target contains $N$ atoms of atomic number $Z$ per $\mathrm{cm}^{3}$. An $\alpha$ particle is deviated at an angle greater than $\theta$ if the approach distance is lower than the impact parameter defined in Eq. (3.5). In this particular target, there are $N \Delta x$ possible circles that the incident particle might encounter. The probability of deviation at an angle greater than $\theta$ is thus given by:

$$
p(\text { deviation } \geq \theta)=\frac{\left(\pi b^{2} N \Delta x\right)_{\left[\mathrm{cm}^{2}\right]}}{1_{\left[\mathrm{cm}^{2}\right]}}=\pi N \Delta x\left(\frac{z Z e^{2}}{4 \pi \varepsilon_{0} m v_{(-\infty)}^{2}}\right)^{2} \operatorname{cotan} \frac{\theta}{2}
$$

By derivation, we obtain:

$$
p(\theta \leq \text { deviation } \leq \theta+d \theta)=\pi N \Delta x\left(\frac{z Z e^{2}}{4 \pi \varepsilon_{0} m v_{(-\infty)}^{2}}\right)^{2} \frac{\operatorname{cotan} \frac{\theta}{2}}{\sin ^{2} \frac{\theta}{2}} d \theta
$$

Per unit of solid angle $d \Omega=2 \pi \sin \theta d \theta$, we arrive at Rutherford's formula:

$$
p(\Omega)=\pi N \Delta x\left(\frac{z Z e^{2}}{4 \pi \varepsilon_{0} m v_{(-\infty)}^{2}}\right)^{2} \frac{1}{4 \sin ^{4} \frac{\theta}{2}}
$$

Rutherford's pupils, Hans Geiger ${ }^{17}$ and Ernest Marsden, ${ }^{18}$ carried out ${ }^{19}$ experiments on the diffusion of alpha particles by a gold foil (and by other metal foils) in

[^61]
(Public domain)
${ }^{18}$ Ernest Marsden (1882-1970). New Zealand physicist. A compatriot of Rutherford, under whom he studied at Manchester, Marsden worked with Geiger on the $\alpha$-particle diffusion experiments. He returned to New Zealand in 1914, where in 1926 he founded the Department of Industrial and Scientific Research. During the Second World War, he worked on the development of radars.

(Public domain)

[^62]1909 at the University of Manchester. These experiments were interpreted with great precision using Rutherford's formula. It was also shown that the probability of deviation remains proportional to thickness, indicating the diffusion remains simple (obviously, provided that the thickness remains low in relation to the stopping distance). Consequently, the impact parameter $b$ is very small in relation to the diameter of the atom and the positive charges concentrated in a nucleus of very small size in relation to that of the atom. This conclusion overturned the atomic model of Thomson. These experiments also showed that the atomic number of the target is approximately equal to $A / 2$, within the series of metals considered, in other words up to lead.

Another extremely interesting conclusion derived from these experiments is the finding of a discrepancy in Rutherford's law, where the angle of diffusion tends towards $\pi=180^{\circ}$, in other words the impact parameter $b$ is very small in the case of a head-on collision where the approach distance is minimal. This finding indicates that at very small approach distances, Coulomb's law no longer applies, in other words that very short-range nuclear forces are able to overcome Coulomb repulsion at distances of less than $10^{-13} \mathrm{~cm}$.

The discrepancy between Rutherford's model and reality is all the greater as the mass of the target decreases. Indeed, in this case, the recoil movement in the target can no longer be ignored, since it absorbs part of the kinetic energy of the projectile and modifies the balances established for a target that is assumed to be fixed. Second, the lower atomic number of the target reduces the Coulomb repulsion, enabling the incident particle to draw closer to the nucleus. In this case, the nuclear force field is more intense, which more clearly demonstrates the limits of Coulomb's law. The effect is thus most marked when the target is hydrogen. Paraffin is a hydrogenated substance perfectly suited for such experiments. Note that firing $\alpha$ particles at a paraffin screen shows that the $\alpha$ particles eject nuclei of hydrogen, thus protons. Indeed, if a source of $\alpha$ particles is placed in the air, scintillation can be seen on a sulfide screen up to source/screen distances of around 20 cm . Beyond this point, all of the $\alpha$ particles are absorbed. However, if a layer of paraffin is placed between the source and the screen near the source, at distances of over 1 m , further scintillation of different type is observed and is caused by radiation historically known as " $H$ rays". These rays are in fact protons ejected by the paraffin. Since the mass of the proton is around four times lower than that of an $\alpha$ particle, the speed of the proton may be up to 1.6 times greater than that of the $\alpha$ particle, resulting in deeper penetration in the air.

### 3.8 Transfer of Energy to Matter

(Valentin 1982a, b, p. 161; Cauchois and Héno 1964, p. 37; Shultis and Faw 2000)
In order to calculate the energy transferred to matter by collisions of particles passing through it, and according to the elastic scattering hypothesis, we can use the results obtained during the study of neutron collisions, namely that speeds of particles before and after interaction are constant in the center-of-mass framework (Fig. 3.33).

Fig. 3.33 Velocity triangle (fixed target)


By projection on $0 x$ :

$$
\begin{gathered}
v_{\otimes} \cos \theta=\frac{m}{M+m} v+v_{\otimes}^{\prime} \cos \Psi \\
\text { avec } v_{\otimes}^{\prime}=\frac{M}{M+m} v \\
\left\{\begin{array}{c}
v_{\otimes} \cos \theta=\left(\frac{m+M \cos \psi}{M+m}\right) v \\
v_{\otimes}^{2}=\left(\frac{M^{2}+2 M m \cos \psi+m^{2}}{(M+m)^{2}}\right) v^{2} \\
\cos \theta=\frac{m+M \cos \psi}{\sqrt{M^{2}+2 M m \cos \psi+m^{2}}} \\
\tan \theta=\frac{v_{\otimes}^{\prime} \sin \Psi}{\frac{m}{m+M} v+v_{\otimes}^{\prime} \cos \Psi}=\frac{\sin \Psi}{\frac{m}{M}+\cos \Psi}
\end{array}\right.
\end{gathered}
$$

By construction, the angle of deviation of the target in the center-of-mass framework, $\pi-\psi$, is equal to twice the angle of deviation of the target in the laboratory framework, denoted $\varphi: \pi-\psi=2 \varphi$. Conservation of the momentum before and after collision in the laboratory framework is written:

$$
m \vec{v}=m \vec{v}_{\otimes}+M \vec{V}_{\otimes}
$$

Projecting onto the $0 x$ axis we have: $(m v)^{2}+\left(M V_{\otimes}\right)^{2}-2 m v M V_{\otimes} \cos \varphi=\left(m v_{\otimes}\right)^{2}$ Conservation of (non-relativistic) kinetic energy is written as:

$$
\frac{1}{2} m v^{2}=\frac{1}{2} m v_{\otimes}^{2}+\frac{1}{2} M V_{\otimes}^{2}
$$

Combining these expressions gives the recoil energy of the target, classically denoted $T=M V_{\otimes}^{2} / 2$ as a function of the initial kinetic energy of the incident particle, $E_{0}=m v^{2} / 2$ (Figs. 3.34 and 3.35):


Fig. 3.34 Elastic scattering at the center of the laboratory model


Fig. 3.35 Elastic scattering at the center of mass

$$
T=\frac{1}{2} M V_{\otimes}^{2}=\frac{4 m M}{(m+M)^{2}} E_{0} \cos ^{2} \varphi=\frac{4 m M}{(m+M)^{2}} E_{0} \sin ^{2} \frac{\psi}{2}
$$

The total kinetic energy available at the center of mass is:

$$
\begin{aligned}
E_{t o t}^{\prime}=\frac{1}{2} m v^{\prime 2}+ & \frac{1}{2} M V^{\prime 2}=\frac{1}{2} m\left(\frac{M v}{M+m}\right)^{2}+\frac{1}{2} M\left(\frac{m v}{M+m}\right)^{2} \\
& =\frac{1}{2} m v^{2} \frac{M}{M+m}=E_{0} \frac{M}{M+m}
\end{aligned}
$$

The minimum approach distance of a charged target is given by the following quality:

$$
\frac{z Z e^{2}}{4 \pi \varepsilon_{0} l}=E_{0} \frac{M}{M+m} \text { thus }: \quad l=\frac{z Z e^{2}(M+m)}{4 \pi \varepsilon_{0} E_{0} M}
$$

The impact parameter is given by:

$$
b=\frac{l}{2 \tan (\psi / 2)}=\frac{z Z e^{2}(M+m)}{8 \pi \varepsilon_{0} E_{0} M \tan (\psi / 2)} .
$$

The differential energy cross section characterizing the probability of energy transfer $T$ to $d T$ is calculated as follows:

$$
\frac{d \sigma}{d T}=\frac{2 \pi b d b}{d T}
$$

Since : $\quad b^{2}=\frac{l^{2}}{4 \tan ^{2}(\psi / 2)}=\frac{l^{2} \cos ^{2}(\psi / 2)}{4 \sin ^{2}(\psi / 2)}=\frac{l^{2}\left(1-\sin ^{2}(\psi / 2)\right)}{4 \sin ^{2}(\psi / 2)}$
we have : $\sin ^{2}(\psi / 2)=\frac{l^{2}}{l^{2}+4 b^{2}}$
giving $T=\frac{4 m M}{(m+M)^{2}} E_{0} \frac{l^{2}}{l^{2}+4 b^{2}}$
the logarithmic derivative of which yields:

$$
\frac{d T}{T}=-\frac{8 b d b}{l^{2}+4 b^{2}}
$$

Finally, given that $d T$ is negative for a collision due to energy loss:

$$
\frac{d \sigma}{d T}=-\frac{\pi l^{2}}{T^{2}} \frac{m M}{(m+M)^{2}} E_{0}
$$

Since $l=\frac{z Z e^{2}(M+m)}{4 \pi \varepsilon_{0} E_{0} M}$, the positive probability is finally given by:

$$
\left|\frac{d \sigma}{d T}\right|=\pi \frac{m M}{(m+M)^{2}} E_{0} \frac{l^{2}}{T^{2}}=\frac{1}{T^{2}} \frac{z^{2} Z^{2} e^{4} m}{16 \pi \varepsilon_{0}^{2} M E_{0}}
$$

A parabola is obtained as a function of the recoil energy $T$, indicating that there is always a greater probability of losing a little energy than of losing a lot of energy. Note that if we compare the probability of collision with an electron ( $Z=1, M=m_{e^{-}}$) or a nucleus ( $Z, M$ ), the ratio of probabilities is given by:

$$
\left(\frac{d \sigma}{d T}\right)_{e^{-}}=\frac{1}{Z^{2}} \frac{M}{m_{e^{-}}}\left(\frac{d \sigma}{d T}\right)_{Z}
$$

Since the electron has a very low mass ( 0.0005 amu ) compared with that of the average nucleus, the probability of interaction with the electron at a given recoil energy is greater for the electron than for the target nucleus. It must be noted that this reasoning assumes a collision, and that the differential energy cross section does not correspond to the pure probability of interaction of the incident particle with the electron or the nucleus. We must also be conscious of the fundamental
calculation hypotheses in which the target is considered immobile at the center of mass prior to the collision. In practice, it is only necessary for the kinetic energy of the electron to be negligible in relation to that of the incident particle, implying that the speed of the particle is not too small compared with that of the orbiting electrons. If the medium crossed has an atomic concentration of $N$ nuclei per $\mathrm{cm}^{3}$ and an atomic number $Z$, the electron density is thus $N Z$, and the number of collisions transferring energy $T$ up to $d T$ per unit length of matter crossed is $N Z d \sigma$. Since every collision by definition transfers an energy of $T$ for an elementary path $d x$, we have (the negative sign indicates energy loss):

$$
-d T=N Z d \sigma T d x
$$

The quantity $R=-d T / d x$ is known as the slowing down power (Berthelot 1956, p. 41), or stopping power, and it has been measured for very many substances and for various charged particles. The elementary transfer must be integrated over all possible transfers between $T_{\min }$ and the quantity:

$$
T_{\max }=\lim _{l \rightarrow+\infty} T=\lim _{l \rightarrow+\infty}\left[\frac{4 m M}{(m+M)^{2}} E_{0} \frac{l^{2}}{l^{2}+4 b^{2}}\right]=\frac{4 m M}{(m+M)^{2}} E_{0}
$$

where, in the present case, $M$ is the mass of the electron $m_{e^{-}}$. Thus, using the differential cross section in relation to the transfer, applied to a target electron:

$$
\begin{aligned}
& \left(\begin{array}{rl}
\left(\frac{d \sigma}{d T}\right)_{\text {electron }}=\left(\frac{1}{T^{2}} \frac{z^{2} Z^{2} e^{4} m}{16 \pi \varepsilon_{0}^{2} M E_{0}}\right)_{\begin{array}{l}
Z \\
M
\end{array}=m_{e^{-}}}=\frac{1}{T^{2}} \frac{z^{2} e^{4} m}{16 \pi \varepsilon_{0}^{2} M E_{0}}
\end{array}\right. \\
& \frac{d T}{d x}=\int_{T_{\min }}^{T_{\max }} N Z d \sigma T=\int_{T_{\min }}^{T_{\max }} N Z T \frac{1}{T^{2}} \frac{z^{2} e^{4} m}{16 \pi \varepsilon_{0}^{2} m_{e^{-}} E_{0}} d T=N Z \frac{z^{2} e^{4} m}{16 \pi \varepsilon_{0}^{2} m_{e^{-}} E_{0}} \ln \left(\frac{T_{\max }}{T_{\min }}\right)
\end{aligned}
$$

Since $E_{0}=\frac{1}{2} m v^{2}$, the mass of the incident particle may be eliminated from the formula:

$$
-\frac{d T}{d x}=N Z \frac{z^{2} e^{4}}{8 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}} \ln \left(\frac{T_{\max }}{T_{\min }}\right)=N Z \frac{z^{2} e^{4}}{4 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}} \ln \left(\frac{T_{\max }}{T_{\min }}\right)^{\frac{1}{2}}
$$

The stopping power $d T / d x$ of a substance is obtained via the atomic number $Z$. It also depends on the incident particle via $z$ and is greater for a massive particle, via $m$. This explains why $\alpha$ particles have very little penetration. The quantity $T_{\min }$, also referred to as the mean ionizing potential, $I$, is the minimum energy required to strip an electron from an atom in the matter being traversed (Cauchois and Héno 1964, p. 52). It can be calculated if we know the level of filling of the last electron shell in which the electrons are less tightly bound according to the formulae seen in Chap. 1. A more
precise analysis involving quantum physics enables this formula to be modified slightly to take into account both the relativistic effects where the speed of the incident particle approaches the speed of light, and the electron structure of the target nucleus by means of a large correction coefficient at low energy $c(E, Z) / Z$ which depends on the energy and the matter being traversed: this is the Bethe-Bloch formula (Fig. 3.36):

$$
-\frac{d T}{d x}=N Z \frac{z^{2} e^{4}}{4 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}}\left[\operatorname{In}\left(\frac{T_{\max }}{T_{\min }}\right)-\ln \left(1-\frac{v^{2}}{c^{2}}\right)-\frac{v^{2}}{c^{2}}-\frac{c(E, Z)}{Z}\right]
$$

It may be seen that the power $1 / 2$ has disappeared from the logarithm (Cahen and Treille 1963, p. 66; Berthelot 1956, p. 120; Lilley 2001, p. 131). If we disregard the mass of the electron in relation to that of the incident particle, which is valid for a proton or an $\alpha$ particle, we obtain:

$$
T_{\max }=\frac{4 m m_{e^{-}}}{\left(m+m_{e^{-}}\right)^{2}} E_{0} \approx \frac{4 m_{e^{-}}}{m} \frac{1}{2} m v^{2}=2 m_{e^{-}-v^{2}}
$$

hence:
Bethe - Bloch formula :

$$
\begin{equation*}
-\frac{d T}{d x}=N Z \frac{z^{2} e^{4}}{4 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}}\left[\ln \left(\frac{2 m_{e^{-}} v^{2}}{I}\right)-\ln \left(1-\frac{v^{2}}{c^{2}}\right)-\frac{v^{2}}{c^{2}}-\frac{c(E, Z)}{Z}\right] \tag{3.6}
\end{equation*}
$$

At very high energies (above 1000 MeV ), it may be seen experimentally that linear energy loss saturates the value known as the Fermi ionization plateau because the very high-speed particle polarizes the medium crossed and forms dipoles whose electromagnetic field opposes that created by the movement of the particle, thereby compensating for the stopping power. It should be noted that


Fig. 3.36 Bethe-Bloch formula as a function of energy of the incident particle
stopping power depends solely on the charge of the incident particle and not on its mass. However, the path followed by charged particles in matter depends both on the $z$ and the mass of the latter. It may be calculated by means of the following formula (taking only the logarithmic term of the Bethe-Bloch formula and using $d T=m v d v$ ):

$$
\begin{aligned}
X & \approx \int_{T=0}^{T=E_{0}} \frac{d x}{d T} d T=\int_{T=0}^{T=E_{0}} \frac{1}{N Z \frac{z^{2} e^{4}}{4 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}}}\left[\ln \left(\frac{2 m_{e^{-}} v^{2}}{I}\right)\right]
\end{aligned} m v d v .
$$

### 3.9 Ion-Electron Pair Production by Ionization

We have seen that the number of collisions between the incident particle and the electrons in substance being crossed is $N Z d \sigma d x$ over a path of $d x$. Where $I_{\text {min }}$ is the minimum ionization energy ( $I$ is the mean energy), the number of electrons receiving energy per unit length is:

$$
\frac{d n_{e^{-}}}{d x}=\int_{T=I_{\min }}^{T=T_{\max }} N Z d \sigma=\int_{T=I_{\min }}^{T=T_{\max }} N Z \frac{1}{T^{2}} \frac{z^{2} e^{4} m}{16 \pi \varepsilon_{0}^{2} m_{e^{-}} E_{0}} d T=N Z \frac{z^{2} e^{4}}{8 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}}\left[\frac{1}{I_{\min }}-\frac{1}{T_{\max }}\right]
$$

This result gives only the number of primary electrons produced by ionization, but the total number of ion pairs created is far higher since the primary electrons speeded up also create ions by virtue of an electromagnetic cascade in which every particle emitted must be followed. The Monte-Carlo codes, which provide a statistical simulation of the path of particles through matter, are extremely useful for this kind of calculation. The order of magnitude of ionization energy necessary to create an ion-electron pair can be calculated using the following formula (again, using only the logarithmic part of the Bethe-Bloch formula):

$$
\begin{aligned}
E_{\text {ionization }} & =\frac{d T}{d n_{e^{-}}}=\frac{\frac{d T}{d x}}{\frac{d n_{e}-}{d x}} \approx \frac{N Z \frac{z^{2} e^{4}}{4 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}}\left[\ln \left(\frac{2 m_{e^{-}} v^{2}}{I}\right)\right]}{N Z \frac{z^{2} e^{4}}{8 \pi \varepsilon_{0}^{2} m_{e^{-}} v^{2}}\left[\frac{1}{I_{\min }}-\frac{1}{T_{\max }}\right]} \approx 2 \frac{\left[\ln \left(\frac{2 m_{e^{-}}{ }^{2}}{I}\right)\right]}{\left[\frac{1}{I_{\min }}-\frac{1}{T_{\max }}\right]} \\
& \approx 2 I_{\min }\left[\ln \left(\frac{2 m_{e^{-}} v^{2}}{I}\right)\right]
\end{aligned}
$$

and disregarding $1 / T_{\max }$ with respect to $1 / I_{\text {min }}$.

### 3.10 Variation in Charge

Charged particles may capture electrons as they pass through matter. Thus, moving protons may capture an electron to become a neutral hydrogen atom that continues along its path from the point of capture tangentially to its initial trajectory deflected by the electromagnetic field (Berthelot 1956, p. 28). The probability of capture of an electron is characterized by the effective capture cross section, $\sigma_{+}$. However, the hydrogen atom thus formed may itself give up at its electron over its own trajectory with a probability of loss of $\sigma_{-}$. Thus, for a beam comprising hydrogen protons and atoms distributed randomly, its distribution of $n_{H} / n_{p}$ will tend towards $\sigma_{+} / \sigma_{-}$after several mean free paths. It has been noted that the charge of a proton at 100 keV changes several hundred times per mm of trajectory through a gas at normal pressure and temperature (Berthelot 1956, p. 34). For $\alpha$ particles, there are three possible states of charge: the neutral atom, ${ }_{2}^{4} \mathrm{He}$, the ion, ${ }_{2}^{4} \mathrm{He}$, and the $\alpha$ particle proper, ${ }_{2}^{4} \mathrm{He}^{2+}$. For the ${ }_{2}^{4} \mathrm{He}^{+}$state, two effective cross sections, one for loss and the other for capture, were measured by Rutherford and Henderson in 1924.

### 3.11 Fission Products

During fission, fission fragments are not necessarily neutral but are ionized. They therefore have an effective charge lower than the $z$ of the neutral isotope. On passing through a medium, fission products may capture a certain number of electrons and the effective charge varies over the trajectory (Berthelot 1956, p. 103). However, the Bethe-Bloch formula is only valid provided there is no variation in the charge on the incident particle. Experimentally, it may be seen that the effective charge is practically independent of the medium being crossed where the latter is thin; however, the effective charge varies during slowing down in the medium. Because of their high mass and speed, fission fragments collide not only with electrons but also with the nuclei of the matter through which they are travelling, and the Bethe-Bloch formula may thus be applied, taking into account the $Z$ protons of the target nucleus. Thus, at the start of travel, Bethe's formula is applicable for collision with electrons, and at the end of travel, only slowing down by protons in the nucleus is important. Finally, the fission products have a very high stopping power and a high capacity for ionizing the medium. In the case of a solid such as uranium, they may be considered as remaining at the point of fission. Subsequently, chemical diffusion phenomena come into play, particularly as a result of the high thermal gradients in the fuel pellet. Atoms of gas such as xenon, which do not bond chemically, migrate towards the porosities, then towards the pellet-cladding gap when these porosities open or when fissures appear in the fuel (Radiation Effect in Refractory Fuel Compounds 1962).

### 3.12 Path Length in Matter

(Bertin 1991)
Because of their mass, $\alpha$ particles are very quickly stopped in matter. It is commonly said that a single sheet of paper is enough to stop $\alpha$ particles at an energy of 5 MeV , which is a good order of magnitude of the energy of $\alpha$ particles involved in decay. For this reason, it is normal to consider that external exposure to $\alpha$ radiation is relatively harmless, since clothing stops these particles completely. The situation involving ingestion or inhalation of $\alpha$ emitters, however, is totally different, since in this case it is human tissue (lungs, stomach) that is irradiated (Hine and Brownell 1956, p. 125). Table 3.3 summarizes the problems at several different orders of magnitude (Boutin 1977, p. 97):

In air at STP (density $\rho=1.310^{-3} \mathrm{~g} / \mathrm{cm}^{3}$, mean atomic mass $A=14.4$ ), the path length of $\alpha$ particles at an energy of between 4 and 10 MeV is given by the following correlation (Foos 1994, p. 138):

$$
R_{[\mathrm{cm}]}=0.32 E_{[\mathrm{MeV}]}^{1.5}
$$

For protons at $10-100 \mathrm{MeV}$, again in air, the following formula may be used:

$$
R_{[\mathrm{cm}]}=1.8 E_{[\mathrm{MeV}]}^{1.8}
$$

Electrons are able to penetrate much more deeply into matter. While less destructive than other particles due to their very low mass, they still require external radioprotection measures (Table 3.4).

The Bragg-Kleeman rule can be used to determine the path length for a charged particle in matter of density $\rho_{2}$ and atomic mass $A_{2}$ where the path length in another substance is known ( $\rho_{1}, A_{1}$ ) (Mayo 1998, p. 273):

Table 3.3 Penetration of matter by $\alpha$ particles

| Energy | Air | Water or living tissue | Aluminum | Lead |
| :--- | :--- | :--- | :--- | :--- |
| 1 MeV | 0.5 cm | $8 \mu \mathrm{~m}$ | $3 \mu \mathrm{~m}$ | $1 \mu \mathrm{~m}$ |
| 5 MeV | 3.5 cm | $45 \mu \mathrm{~m}$ | $21 \mu \mathrm{~m}$ | $7 \mu \mathrm{~m}$ |

Table 3.4 Penetration of matter by electrons

| Energy | Air | Water or living tissue | Aluminum | Lead |
| :--- | :--- | :--- | :--- | :--- |
| 1 MeV | 3 m | 4 mm | 1.5 mm | 0.35 mm |
| 3 MeV | 10 m | 15 mm | 5.5 mm | 1.3 mm |

Table 3.5 Half-value layer for photons in matter

| Energy | Air | Water and living tissue | Concrete | Lead |
| :--- | :--- | :--- | :--- | :--- |
| 1 MeV | 150 m | 15 cm | 6 cm | 1.5 cm |

Bragg - Kleeman rule for penetration distances : $\quad \frac{R_{2}}{R_{1}}=\frac{\rho_{2}}{\rho_{1}} \sqrt{\frac{A_{1}}{A_{2}}}$
Care should be taken not to invert atomic mass indices and densities. Photons are by far the most penetrative particles and are better attenuated by heavy screens (such as lead). The value generally used is the half-value layer (HVL), which is the length over which the intensity of the photon beam is halved (Table 3.5):

In order to eliminate all danger, attenuation is generally multiplied by a coefficient of 1000 , i.e. around $10 \mathrm{HVL}\left(2^{10}=1024\right)$. While the path length in matter of the heaviest ions is even lower than that of $\alpha$ particles, they cause far more damage. An ion flux on a surface may even result in a certain degree of sputtering (abrasion) of the latter (Atomic Collisions in Solids 1976). Such abrasion occurs, though more weakly, for less massive particles such as neutrons and electrons. The science of radioprotection, as utilized for the safety of staff working in the vicinity of natural or artificial radioactivity, provides simple tables for the standard cases as well as precise calculation codes for more complex situations [e.g. travel of particles around obstacles via reflection (Rockwell 1956, p. 316), use of holes as particle guides (Rockwell 1956, p. 261), etc.], thus enabling effective determination of the actual protection required (Baur 1985; Berthelot 1956; Delacroix et al. 2006; Harrison 1958; Métivier 2006).

### 3.13 Biological Effects of Radiation

Various types of biological damage may be caused by ionizing radiation and these depend essentially on linear energy transfer (LET, usually expressed in $\mathrm{keV} \mu \mathrm{m}^{-1}$ ). Radiation at a high LET causes multiple lesions, primarily along the trajectory of the particle, but also around this trajectory due to the appearance of secondary particles (cascade effects). Sensitive impact sites include the cytoplasmic membrane and nucleus of cells. In particular, incident particles can cause damage (Fig. 3.37) to strands of deoxyribonucleic acid (DNA) bearing genetic information. Damage can occur by direct impact of the particle on DNA, but also by thermalchemical effects due to the radiolysis of water molecules immediately surrounding the DNA (with the appearance of "aggressive" free radicals). It should be noted that in the case of neutrons, the problems arise more from the risk of protons being ejected by neutrons since these charged protons interact strongly with matter and have a high potential for secondary ionization with strong energy deposition.

To give an idea of the order of magnitude, it is estimated that a low-LET particle depositing energy of 1 Gray in a cell produces 500-1000 single-strand breaks in DNA and 40 double-strand breaks. Such breaks are partially repaired by a

Fig. 3.37 Effects of radiation on DNA [adapted from Poretti (1988)]

continuous process, but they may be duplicated during cell division, with risk of chromosomal mutation or aberration. Edwards' formula (1990) correlates the number of observed aberrations $A b$ to dose $G$ (in Gray) using a quadratic equation:

$$
A b=a+b G+c G^{2}
$$

The coefficients of this equation depend on the radiation type (neutrons, photons, etc.), and, to a lesser extent, on the dose rate, as shown in Fig. 3.38. Following accidental irradiation, this method of analysis may be used to determine the
absorbed dose by analyzing the number of aberrations in blood. We can see that different types of radiation do not create the same amount of damage for the same dose received, which is why the concept of dose equivalent is used.

The relative biological effectiveness ( RBE ) is the ratio between the absorbed dose and a reference dose required to produce the same biological effect. RBE thus corresponds to a given biological effect such as cell survival (Fig. 3.39). The

Fig. 3.38 Frequency of dicentric chromosome aberrations (the broken ends of a damaged chromosome join up with an intact chromosome) as a function of the dose induced by neutrons at 1.1 MeV or by photons resulting from the decay of cobalt 60, after P. Versin (P. Versin: Effets biologiques des neutrons, mécanismes et applications [Biological effects of neutrons: mechanisms and applications],
Radioprotection Vol. 34, No 4, pp 521-543, 1999)

Fig. 3.39 Relative biological efficiency as a function of TLE in relation to human cell survival under normal conditions and in hypoxia (lack of oxygen). The effective cross sections correspond to the quadratic cell survival curve for a lethal dose (adapted from Barendsen 1997) (G. W. Barendsen: Parameters of linear-quadratic radiation dose effect relationships dependence on LET and mechanisms of reproductive cell death, J. Radiat. Biology, 71, pp. 649-655, 1997)

standard reference radiation is that produced by cobalt 60 , or high-energy x-rays. RBE is dependent on LET as well as the absorbed dose. For neutrons, the RBE is maximal for an energy of around 0.5 MeV as regards animal cells. Overall, the effects of neutrons are more serious than those of x-rays or photons of lower LET, which, although problematic in the event of accidental irradiation, may constitute an advantage in local radiotherapy.

## Chapter 4 <br> Neutron Slowing-Down

### 4.1 Historical Background

(Bernardini and Bonolis 2004; Génie de la science $n^{\circ} 6$ 2001)
Neutron slowing-down was established at the end of the 1930s by Enrico Fermi. He worked on several research areas in theoretical physics such as the behavior of ideal gases based on a quantum statistical approach from 1925 to 1927, producing the Fermi gas model (Greiner et al. 1999, p389), and on $\beta$ radioactive decay in 1933, for which he was awarded the Nobel Prize. In 1934, he began working on artificial radioactivity discovered by Frédéric and Irène Joliot-Curie. With his Roman team composed of Emilio Segrè, ${ }^{1}$ Edoardo Amaldi, ${ }^{2}$ Franco Rasetti ${ }^{3}$ and Oscar D'Agostino, ${ }^{4}$ he worked on the bombardment of several targets by neutrons. Rutherford, who was quite contemptuous of pure theorists, congratulated him for

[^63]

Photo 4.1 The Italian team: from left to right D'Agostino, Emilio Segré, Edoardo Amaldi, Franco Rasetti and Enrico Fermi (University of Rome)
crossing the line into experimental work. One morning, according to Laura Fermi, his wife, Emilio Segrè was sent out with a shopping basket to buy all of the pure elements that could then be bought in pharmacy stores. While the experiments on light elements produced nothing, for heavier nuclei, Fermi and his team obtained artificial radioactivity in large quantities (Photo 4.1).

While investigating optimum conditions for neutron capture, Edoardo Amaldi and Bruno Pontecorvo ${ }^{5}$ observed a strange phenomenon. They placed a neutron source inside a silver cylinder for irradiation, the cylinder being itself inside a lead casket. Quite surprisingly, the induced activity differed depending on whether the cylinder was in the center or in a corner of the casket. Fermi suggested irradiating the external surface of the cylinder and they observed that nearby objects influenced the activity of the radioactive silver produced during the experiment. Even stranger was the fact that when the cylinder was placed on a wooden table, the activity was intense, whereas on the marble chemistry bench, it was weak. Intrigued by this

[^64]effect, the experimenters dubbed the wooden table a "magic table". On October 20, 1934, they decided to remove the neutron source from the cylinder and place it next to the cylinder, with a thin sheet of lead inserted between the two in order to differentiate between absorbed neutrons and those scattered by the lead. In a flash of inspiration, Fermi replaced the lead casket with a paraffin block (Photo 4.2).

The paraffin block very significantly increased the induced activity of the silver. Fermi immediately proposed a physical explanation: the paraffin slowed down the


Photo 4.2 Although Enrico Fermi (1901-1954) is not well-known to the general public, the French magazine "Les génies de la science" ['Geniuses of science'] published an excellent article in his honor. Although several attempts were made to name a unit of length after him (one Fermi is equal to one femtometer), this was never a success, doubtless because $F$ is already the symbol for the farad, the unit of capacitance in electromagnetism (courtesy Belin)
neutrons, rendering them more "effective". Thus, the induced activity was inversely proportional to neutron speed. Fermi discovered that capture cross sections have a $1 / v$ shape. The experimental apparatus was immediately set up in the fountain, with its goldfish, in front of the Institute. The result was identical: just like paraffin, hydrogen-rich water increased the induced activity by slowing down the neutrons. The collision of neutrons with light atoms in paraffin or water causes the sloweddown neutrons to be captured with maximum efficiency. This work on neutron properties continued until 1936, when the Italian political climate worsened dramatically. Indeed, Mussolini's fascist movement was now at the height of its power thanks to its agreements concluded with Germany. The Second World War eventually disrupted Italian science. Let us return, however, to Fermi's team: they bombarded different substances in rising order of mass and finally came to uranium. However, the large number of radioactive products observed prevented Fermi from understanding uranium fission (an unthinkable feat at that time!). In an unfortunate experiment, Amaldi failed to detect recoil fission products due to an aluminum foil that created a barrier and prevented these products from entering the ionization chamber. Hahn and Strassman discovered uranium fission in 1939 using chemical methods.

The initial energy of a neutron created immediately after fission is distributed according to a fast spectrum $\chi(E)$ given by several semi-empirical formulae (e.g. Watt spectrum) and has a mean value of 2 MeV . The neutron travels through matter and may eventually collide with a ${ }_{92}^{238} U$ nucleus, which may in turn undergo fission. Otherwise, the neutron loses energy during the slowing-down phase, in which successive collisions cause energy loss in a discontinuous fashion. These collisions are initially inelastic and anisotropic but they become elastic and isotropic as the speed of the neutron decreases. At high energies ( $>0.8 \mathrm{MeV}$ ), the capture cross sections are small and many neutrons are able to survive this primary slowingdown phase. Between 50 keV and 5 keV , few captures occur and all collisions are now elastic and virtually isotropic in the center of mass. Below 5 keV , the neutron passes through the resonance region of the various cross sections, namely those of ${ }_{92}^{238} U$, where its probability of capture greatly increases. If it survives below this energy, it reaches the thermal domain in which absorption becomes more probable as its speed decreases ( $1 / v$ law). The speed of the neutron then reaches thermal equilibrium with Brownian motion of the medium (with a mean energy of $k T=0.0253 \mathrm{eV}$ for a medium at $20.44{ }^{\circ} \mathrm{C}$ ): this is the thermalization phase in which the neutron may gain energy by collision with "hot" matter.

### 4.2 Continuous-Energy Slowing-Down Theory

(Glasstone and Edlund 1972, p137; Baur 1985, p141; Mayo 1998, p110; Soodak 1962, p121; Ferziger and Zweifel 1966, p47)

Fig. 4.1 Triangle for velocity composition: $\theta$ is the scattering angle in the laboratory frame, and $\Psi$ the corresponding angle in the center-of-mass frame


### 4.2.1 Elastic Collision with a Stationary Target

The laws of elastic collision, seen earlier in the chapter on neutron interaction with matter, enable calculation of the energy, $E_{1}$ (in the laboratory frame), of a neutron (initial energy $E_{0}$ ) after it has collided with a target of mass $A$, and where the neutron mass is 1 unit:

Energy loss in the laboratory frame : $E_{1}=E_{0}\left(\frac{A^{2}+1}{(A+1)^{2}}+\frac{2 A}{(A+1)^{2}} \cos \Psi\right)$
as a function of the scattering angle in the center of mass (Fig. 4.1).

$$
\text { Using }^{6} \alpha \equiv\left(\frac{A-1}{A+1}\right)^{2},
$$

$$
E_{1}=\frac{E_{0}}{2}[(1+\alpha)+(1-\alpha) \cos \Psi]
$$

The speed $v_{1}$ of the neutron after collision in the laboratory frame is given by:

$$
\begin{equation*}
\frac{v_{1}^{2}}{v_{0}^{2}}=\frac{A^{2}+1+2 A \cos \Psi}{(A+1)^{2}} \tag{4.2}
\end{equation*}
$$

By vector composition: $\overrightarrow{v_{1}}=\overrightarrow{v_{1 \otimes}}+\frac{1}{A+1} \overrightarrow{v_{0}}$ and $v_{0 \otimes}=v_{1 \otimes}$.
By projection on the $x$-axis, the cosine of the scattering angle $\theta$ in the laboratory frame may be computed:

[^65]$$
v_{1} \cos \theta=\frac{A}{A+1} v_{0} \cos \psi+\frac{1}{A+1} v_{0}
$$

Using Eq. (4.2):

$$
\begin{equation*}
\cos \theta=\frac{A+1}{2} \frac{v_{1}}{v_{0}}-\frac{A-1}{2} \frac{v_{0}}{v_{1}} \tag{4.3}
\end{equation*}
$$

and:

$$
\begin{equation*}
\cos \psi=1-\frac{(A+1)^{2}}{2 A}\left[1-\left(\frac{v_{0}}{v_{1}}\right)^{2}\right] \tag{4.4}
\end{equation*}
$$

These equations show that maximum energy loss occurs when $\Psi=\pi$ (head-on collision with the neutron is reflected in the opposite direction) and minimum energy loss occurs when $\Psi=0$ (tangential collision with a neutron, which continues in the same direction). Since collisions are random events, it is interesting to compute the mean energy loss per collision. Let $P(E)$ be the probability of obtaining the energy $E=E_{0}[(1+\alpha)+(1-\alpha) \cos \Psi] / 2$ after the collision. Thus:

$$
d E=-\frac{E_{0}}{2}(1-\alpha) \sin \Psi d \Psi \quad \Rightarrow \quad-d(\cos \Psi)=\frac{2 d E}{E_{0}(1-\alpha)}
$$

If the collision is isotropic in the center of mass, which is the case at low energy, all scattering directions are equiprobable and the probability of a neutron scattering in a direction $\Psi$ to $d \Psi$ is equivalent to the proportion of the solid angle ${ }^{7}$ :

$$
P(\Psi) d \Psi=\frac{d \Omega}{4 \pi}=\frac{2 \pi \sin \Psi d \Psi}{4 \pi}=\frac{\sin \Psi}{2} d \Psi=-\frac{d(\cos \Psi)}{2}
$$

Since $P(E) d E=P(\Psi) d \Psi: P(E) d E=\frac{d E}{E_{0}(1-\alpha)}$
The energy after collision is always between $\alpha E_{0}$ and $E_{0}$. For hydrogen $(\alpha=0)$, the neutron may lose all its incident energy. This is the equivalent of a "stop-shot" in pool for balls of the same mass. Thus, the neutron has zero probability of having an energy below $\alpha E_{0}$ but a constant probability of an energy between $\alpha E_{0}$ and $E_{0}$. This probability is normalized to 1 as:

$$
\int_{0}^{E_{0}} P(E) d E=\int_{\alpha E_{0}}^{E_{0}} P(E) d E=1
$$

[^66]

Fig. 4.2 Isotropic collision in the center of mass


Fig. 4.3 Probability of reaching energy $E$ and change of variable to lethargy gain

The mean energy of the neutron after collision is (Fig. 4.2):

$$
\int_{\alpha E_{0}}^{E_{0}} E P(E) d E=\int_{\alpha E_{0}}^{E_{0}} \frac{E}{E_{0}(1-\alpha)} d E=\frac{E_{0}^{2}\left(1-\alpha^{2}\right)}{2 E_{0}(1-\alpha)}=\frac{1+\alpha}{2} E_{0}
$$

We thus see that the probability of reaching energy $E$ depends on the initial pre-collision energy, $E_{0}$. A change of variable helps to avoid this problem. Lethargy, $u$, is defined as the dimensionless quantity such that (Fig. 4.3):

$$
\begin{equation*}
\text { Definition of lethargy : } \quad u_{[-]} \equiv \ln \frac{E_{r e f}}{E}=2 \ln \frac{v_{r e f}}{v} \tag{4.5}
\end{equation*}
$$

Lethargy increases as energy decreases (during successive collisions) and is zero for a chosen reference energy $E_{r e f}$. The latter may be equal to $E_{0}$ which is the energy of a neutron at the beginning of its life, before any collisions occur. To obtain only positive values of lethargy, the reference energy may be taken as the maximum
energy of neutrons emitted by fission, i.e. around 10 MeV . Thus a change in lethargy between two successive collisions (or lethargy gain for a collision that decreases the energy of the neutron) is computed as follows:

$$
\begin{aligned}
w \equiv \Delta u= & \ln \frac{E_{0}}{E_{2}}-\ln \frac{E_{0}}{E_{1}}=\ln \frac{E_{1}}{\frac{E_{1}}{2}[(1+\alpha)+(1-\alpha) \cos \Psi]} \\
& =\ln \frac{2}{(1+\alpha)+(1-\alpha) \cos \Psi}
\end{aligned}
$$

The lethargy gain between two collisions here depends solely on $\alpha$ and $\Psi$, and no longer on the initial neutron energy. This is because the post-collision energy remains proportional to the pre-collision energy. Fermi used this feature to tackle the problem in logarithmic terms. If the variable is changed to express the equation $P(E)$ as lethargy, the following is obtained:

$$
P(E) d E=\frac{d E}{E_{0}(1-\alpha)}=\frac{-E_{0} e^{-u} d u}{E_{0}(1-\alpha)}=-\frac{1}{1-\alpha} e^{-u} d u=P(u) d u
$$

It should be noted that during a collision, $d E$ is negative when $d u$ is positive and vice versa. The positive probability of reaching lethargy $u$, up to $d u$, is given by $P(u)=e^{-u} /(1-\alpha)$. By extension, the probability of reaching an increment in lethargy of $w$ up to $d w$ is given by $P(w)=e^{-w} /(1-\alpha)$. The maximum lethargy gain $\varepsilon$ is:

Maximum lethargy gain per collision :

$$
\begin{equation*}
\varepsilon \equiv w_{\max }=u\left(\alpha E_{0}\right)-u\left(E_{0}\right)=\ln \frac{E_{0}}{\alpha E_{0}}=\ln \frac{1}{\alpha} \tag{4.6}
\end{equation*}
$$

The average lethargy gain $\xi$, also called the slowing-down parameter, is defined as:

Average lethargy gain per collision :

$$
\begin{equation*}
\xi \equiv \bar{w}=\int_{0}^{\varepsilon} w P(w) d w=\int_{0}^{\varepsilon} \frac{w}{1-\alpha} e^{-w} d w=1-\frac{\alpha}{1-\alpha} \ln \frac{1}{\alpha} \tag{4.7}
\end{equation*}
$$

The mean square value of the lethargy gain (second moment), which is used in some slowing-down models, is computed as:

$$
\begin{aligned}
\overline{w^{2}} & \equiv \int_{0}^{\varepsilon} w^{2} P(w) d w=\int_{0}^{\varepsilon} \frac{w^{2}}{1-\alpha} e^{-w} d w=\frac{1}{1-\alpha}\left(\left[-w^{2} e^{-w}\right]_{0}^{\varepsilon}+2 \int_{0}^{\varepsilon} w e^{-w} d w\right) \\
& =-\frac{\alpha}{1-\alpha}\left(\ln \frac{1}{\alpha}\right)^{2}+2 \xi
\end{aligned}
$$

from which the derivative, which characterizes the second moment, may be deduced (Meghreblian and Holmes 1960, p104):

$$
\gamma \equiv \frac{\overline{w^{2}}}{2 \xi}=1-\frac{\alpha}{2\left(1-\alpha-\alpha \ln \frac{1}{\alpha}\right)}\left(\ln \frac{1}{\alpha}\right)^{2}=1-\left(\frac{\alpha}{1-\alpha}\right) \frac{\varepsilon^{2}}{2 \xi}
$$

This parameter is also used in some slowing-down models. When the mass of the target increases, the following Taylor-series expansion may be expressed (Fig. 4.4):

$$
\begin{gathered}
\alpha=\left(\frac{A-1}{A+1}\right)^{2} \approx 1-\frac{4}{A}+O\left(\frac{1}{A^{2}}\right) \quad \frac{\alpha}{1-\alpha}=\frac{A}{4}\left(1-\frac{1}{A}\right)^{2} \\
\ln \frac{1}{\alpha}=\ln \left(\frac{A+1}{A-1}\right)^{2}=2 \ln \left[\left(1+\frac{1}{A}\right)\left(1+\frac{1}{A}+\frac{1}{A^{2}}+O\left(\frac{1}{A^{3}}\right)\right)\right] \approx \frac{4}{A}\left(1+\frac{1}{3 A^{2}}\right)+O\left(\frac{1}{A^{4}}\right) \\
\left\{\begin{array}{l}
\xi=1-\frac{\alpha}{1-\alpha} \ln \frac{1}{\alpha} \approx 1-\left(1-\frac{1}{A}\right)^{2}\left(1+\frac{1}{3 A^{2}}\right) \approx \frac{2}{A}\left(1-\frac{2}{3 A}\right)+O\left(\frac{1}{A^{3}}\right) \\
\gamma=1-\frac{\alpha}{2 \xi}\left(\ln \frac{1}{\alpha}\right)^{2} \approx 1-\frac{\left(1-\frac{1}{A}\right)^{2}\left(1-\frac{2}{A^{2}}\right)^{2}}{1-\frac{2}{3 A}} \approx \frac{4}{3 A}-\frac{1}{3 A^{2}}+O\left(\frac{1}{A^{3}}\right) \\
\varepsilon=\ln \frac{1}{\alpha} \approx \frac{4}{A}+\frac{4}{3 A^{3}}+O\left(\frac{1}{A^{5}}\right)
\end{array}\right.
\end{gathered}
$$

Hence, thanks to the mean lethargy gain per collision, Fig. 4.5 is interpreted by assuming that if energy loss is plotted on a logarithmic scale, the height of each step is almost constant and equal to $\xi$ (Glasstone and Edlund 1972, p173; Stephenson 1954, p137; Meghreblian and Holmes 1960, p87). Further, the time interval between successive collisions increases since the speed of the neutron decreases

Fig. 4.4 Effect of mass number (via $\alpha$ ) on mean lethargy gain $\xi$ and secondorder moment) $\gamma$



Fig. 4.5 Evolution of a fission neutron versus time

Table 4.1 Average number of collisions required to thermalize a 2 MeV fast neutron

|  | ${ }_{1}^{1} \mathrm{H}$ | ${ }_{1}^{2} \mathrm{H}$ | ${ }_{6}^{12} \mathrm{C}$ | ${ }_{8}^{16} \mathrm{O}$ | ${ }_{11}^{23} \mathrm{Na}$ | ${ }_{92}^{238} \mathrm{U}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Collision at a right angle | 27 | 31 | 121 | 157 | 222 | 2200 |
| $\Delta u / \xi$ | 18 | 25 | 115 | 153 | 205 | 2146 |

significantly. Fermi's original idea consisted in transforming a discrete problem into a continuous one, enabling the use of more advanced mathematical tools (derivation, integration, etc.) for the slowing-down equations. In practice, assuming that all neutrons are born at an energy of 2 MeV and slow down to 0.0253 eV , the number of lethargy units gained is given by (Ligou 1982, p103) (Table 4.1):

$$
\Delta u=\ln \frac{210^{6}}{0.0253}=18.18 \text { lethargy units }
$$

Thus, we may now modify Table 2.2, Chap. 2, in which only collisions at a right angle (at the center of mass) were considered. This concept was used to compute the mean number of collisions required to thermalize a fast neutron of 2 MeV , but this value may now be computed more accurately using $\Delta u / \xi$ :

The exact calculation $(\Delta u / \xi)$ shows that the simplifying hypothesis of a collision at a right angle overestimates the number of collisions required, especially if the latter is small, though it remains representative. The slowing-down parameter $\xi$ for an isotope is constant, although the materials used are often chemical compounds, which are themselves composed of an isotopic mix of varying abundances. If the slowing-down medium is a compound (e.g. light water $\mathrm{H}_{2} \mathrm{O}$, heavy water $\mathrm{D}_{2} \mathrm{O}$,
beryllium oxide BeO ), the average slowing-down parameter $\bar{\xi}$ is defined through weighting of the slowing-down power $\xi \Sigma_{s}$ :

$$
\bar{\xi}(E) \equiv \quad \sum \quad \frac{\xi_{i} \Sigma_{S}^{i}(E)}{\Sigma_{S \text { total }}(E)}
$$

## Nuclide $i \in$ material

While $\xi_{i}$ is energy-independent, $\bar{\xi}$ depends (unfortunately for the simplicity of the model) on $E$ through the terms $\Sigma_{S}^{i}(E)$ and $\Sigma_{S \text { total }}(E)=\sum \Sigma_{S}^{i}(E)$ (Ligou 1982, p106). The second-order moment is weighted as follows:

$$
\bar{\gamma}(E) \equiv \frac{\sum_{i} \gamma_{i} \xi_{i} \Sigma_{S}^{i}(E)}{\sum_{i} \xi_{i} \Sigma_{S}^{i}(E)}
$$

However, the slowing-down power characterizes only the ability to slow down neutrons in a scattering collision. In reality, absorption by a medium reduces its moderating capacity. This is the case for light water for instance, in which the isotope ${ }_{1}^{1} H$ has the best possible $\xi$ value $(\sim 1)$, but which is far more absorbing than deuterium ${ }_{1}^{2} \mathrm{H}$, which is preponderant in heavy water but has a $25 \%$ lower $\xi$. Ultimately, heavy water is a far better moderator than light water, since it is far more absorbing. Thus, the neutron-moderating capacity of a medium may be characterized by its specific slowing-down power ${ }^{8}$ :

$$
\begin{equation*}
\text { Specific slowing-down power : } \quad r \equiv \frac{\xi \Sigma_{S}}{\Sigma_{a}} \tag{4.8}
\end{equation*}
$$

The specific slowing-down power characterizes a moderator by taking into account both the number of scattering atoms, $N_{s}$ (through the term $\xi \Sigma_{S}=\xi N_{s} \sigma_{s}$ ), and the number of absorbing atoms, $N_{a}$, present. These atoms may in fact be the same. This ratio is around 70 for light water but is greater than 20,000 for heavy water! Table 4.2 summarizes the properties of the various moderators used in the nuclear industry. It should be noted in particular that a light-water reactor cannot become critical with natural uranium $\left(0.711 \%\right.$ of $\left.{ }_{92}^{235} U\right)$, and that enrichment in ${ }_{92}^{235} U$ is thus essential. The moderation ratio is characteristic of a specific neutronic situation involving the juxtaposition of some fuel and a moderator. Some authors calculate this ratio using the same formula as for the specific slowing-down power, with an additional term in the denominator to allow for the absorbing nuclides of the fuel, at the risk of confusion with specific-slowing down power. Consequently, this ratio is itself proportional to the ratio of the volumes of water to fuel for a water

[^67]Table 4.2 Different industrial moderators [see also (Lamarsh and Baratta 2001, p317) and (GA Vol. 1, 1967, p210)]

| Moderator | Formula | State | Slowing down $\xi \Sigma_{s\left[\mathrm{~cm}^{-1}\right]}$ | Capture $\sum_{a\left[\mathrm{~cm}^{-1}\right]}$ | $\xi \Sigma_{S} / \Sigma_{a[-]}$ | Cost | Natural U |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Water (298 K) | $\mathrm{H}_{2} \mathrm{O}$ | Liquid | 1.5 | 0.02 | 75 | Zero | Impossible |
| Heavy water | $\mathrm{D}_{2} \mathrm{O}$ | Liquid | 0.18 | 0.000008 | 22,500 | High | Possible |
| Beryllia | BeO | Solid | 0.15 | 0.001 | 150 | Moderate | Possible |
| Graphite | C | Solid | 0.063 | 0.0004 | 157 | Moderate | Possible |

Fig. 4.6 Comparison of the relative spectra for different fast reactors (W. Häfele, D. Faude, A. Fischer, H. Laue: Fast Breeder Reactors, Annual review of Nuclear Science, Annual Reviews, Inc., Palo Alto, California, 1970. Reviewed in (Walter and Reynolds 1981, p132).)

reactor, which is generally termed the technological moderation ratio. For this reason, we prefer to use the term "moderation ratio" to describe the ratio of a volume of water to a volume of fuel.

In industrial reactors, light nuclei adversely affect the fast spectrum of fission neutrons. Therefore, in fast reactors, oxygen from oxide fuel, carbon from carbide fuel and steam from steam-cooled reactors thermalize the energy spectrum to a greater or less extent depending on the moderation ratio. Clearly, this thermalization effect is not desired in fast reactors; it is in fact an automatic consequence of the fuel technology involving light nuclei (Fig. 4.6). It can be seen that reactors with metallic fuel have a faster spectrum.

### 4.2.2 Collision Statistics

During successive collisions, the probability of a neutron of reaching lethargy $u$ after two collisions is:

$$
P_{2}(u)=\int_{u-\varepsilon \leq u^{\prime} \leq u} P_{1}\left(u^{\prime}\right) P\left(u-u^{\prime}\right) d u^{\prime}
$$

where: $P(u) d u=e^{-u} d u /(1-\alpha)$. Note that if all neutrons are assumed to be emitted at a single lethargy, chosen as the origin of lethargies, then $P_{1}(u) \equiv P(u)$. The probability of a neutron reaching $u$ after $n$ collisions is obtained by recurrence:

$$
P_{n}(u)=\int_{u^{\prime}<u} P_{n-1}\left(u^{\prime}\right) P\left(u-u^{\prime}\right) d u^{\prime}
$$

This equation clearly expresses $P_{n}$ as a multiple convolution of $P$. If $u>n \varepsilon$, $P_{n}(u)=0$ since $\varepsilon$ is the maximum lethargy gain for a collision. The probability of exceeding lethargy $u$ after $n$ collisions is calculated by integrating $P_{n}$ over lethargies larger than $u$ :

$$
\Pi_{n}(u) \equiv \int_{u}^{+\infty} P_{n}\left(u^{\prime}\right) d u^{\prime}
$$

This probability indicates the number of neutrons which cross the lethargy $u$ after exactly $n$ collisions. Note that certain of these neutrons will have already exceeded $u$ after $n-1$ collisions. The latter are, thus, characterized by the probability $\Pi_{n-1}(u)$, hence $\mathrm{N}(u)$ is the probability of reaching $u$ after exactly $n$ collisions:

$$
\mathrm{N}(u)=\Pi_{n}(u)-\Pi_{n-1}(u)
$$

This probability enables us to calculate the mean number of collisions required to exceed lethargy $u$ by summing the number of collisions weighted by their occurrence probability:

$$
\begin{equation*}
\text { Mean number of collisions to reach } u: \quad \overline{n(u)}=\sum_{n=1}^{+\infty} n \mathrm{~N}(u) \tag{4.9}
\end{equation*}
$$

Since $P_{n}$ is a convolution, its Laplace transform ${ }^{9}$ is easily computed as the product of its respective images. Using the mathematical notations of (Abramowitz and Stegun 1972) where the Laplace transform $\mathrm{F}(s)$ of a function $f(u)$ is:

[^68]$$
\mathrm{F}(s)=\int_{0}^{+\infty} e^{-s u} f(u) d u
$$
we get:
$$
p(s)=\int_{0}^{+\infty} e^{-s u} \frac{1}{1-\alpha} e^{-u} d u=\frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}
$$
and:
$$
p_{n}(s)=\left[\frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}\right]^{n}
$$

By composition:

$$
\begin{aligned}
& \mathrm{n}(s)=\int_{0}^{+\infty} e^{-s u} \mathrm{~N}(u) d u=\frac{1}{s}\left(\left[\frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}\right]^{n-1}-\left[\frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}\right]^{n}\right) \\
& \quad=\frac{1}{s} \frac{\alpha^{s+1}+(1-\alpha)(s+1)-1}{(1-\alpha)(s+1)}\left[\frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}\right]^{n-1}=\frac{1}{s} \varpi^{n-1}(1-\varpi)
\end{aligned}
$$

using: $\varpi=\frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}$.
The Laplace transform (or image) of the average number of neutrons which exceed $u$ is given by:

$$
\bar{n}(s)=\sum_{n=1}^{+\infty} n \mathrm{n}(s)=\frac{1}{s} \sum_{n=1}^{+\infty} n \varpi^{n-1}(1-\varpi)
$$

This is a series expansion of $\frac{1}{(1-x)^{2}}=\sum_{n=1}^{+\infty} n x^{n-1}$, thus:
Image of the average number of collisions to exceed $u$ :

$$
\begin{equation*}
\bar{n}(s)=\frac{1}{s} \frac{1}{(1-\varpi)}=\frac{1}{s} \frac{(1-\alpha)(s+1)}{\alpha^{s+1}+(1-\alpha)(s+1)-1} \tag{4.10}
\end{equation*}
$$

This image will be later used to compute the neutron flux. The neutron spectrum $\varphi_{n}(E)$ after $n$ collisions may be expressed for hydrogen as:

$$
\left\{\begin{array}{l}
\varphi_{0}(E)=\delta\left(E-E_{0}\right) \\
\varphi_{n}(E)=\frac{1}{E_{0}(n-1)!} \ln ^{n-1}\left(\frac{E}{E_{0}}\right) \quad\left\{\begin{array}{l}
\varphi_{0}(u)=\delta(u) \\
\varphi_{n}(u)=\frac{1}{(n-1)!} e^{-u} u^{n-1}
\end{array}\right. \text {. }
\end{array}\right.
$$

For a nuclide of mass $>1$ :

$$
\varphi_{n}(E)=\int_{E}^{E / \alpha} \frac{\varphi_{n-1}\left(E^{\prime}\right)}{(1-\alpha) E^{\prime}} d E^{\prime} \quad \varphi_{n}(u)=\int_{0}^{\min (u, \varepsilon)} \frac{\varphi_{n-1}\left(u-u^{\prime}\right) e^{-u^{\prime}}}{(1-\alpha)} d u^{\prime}
$$

It should be noted that $\varphi_{n}(u)$ is the probability density for a given $n$ at a given value of $u$, and a discrete probability for a given $u$ at a given value of $n .{ }^{10}$ For a mixture of hydrogen and a heavier nuclide $X$ characterized by its $\alpha$, the neutron spectrum is written as (with the Heaviside function $\Theta$ ):

$$
\left\{\begin{array}{l}
\varphi_{0}(u)=\delta(u) \\
\varphi_{1}(u)=\frac{\Sigma_{s}^{H}}{\Sigma_{s}^{H}+\Sigma_{s}^{X}} e^{-u}+\frac{\Sigma_{s}^{X}}{\Sigma_{s}^{H}+\Sigma_{s}^{X}} \frac{e^{-u} \Theta(\varepsilon-u)}{1-\alpha} \\
\varphi_{n}(u)=\frac{\Sigma_{s}^{H}}{\Sigma_{s}^{H}+\Sigma_{s}^{X}} \int_{0}^{u} \varphi_{n-1}\left(u-u^{\prime}\right) e^{-u^{\prime}} d u^{\prime}+\frac{\Sigma_{s}^{X}}{\Sigma_{s}^{H}+\Sigma_{s}^{X}} \int_{0}^{\min (u, \varepsilon)} \frac{\varphi_{n-1}\left(u-u^{\prime}\right) e^{-u^{\prime}}}{(1-\alpha)} d u^{\prime}
\end{array}\right.
$$

Some authors, e.g. Lamarsh, have insisted on the fact that $n=\langle u / \xi\rangle=\left\langle\frac{\ln \left(E_{0} / E\right)}{\xi}\right\rangle$ is not the average number of collisions required to reach energy $E$ but rather the number of collisions required to gain a mean lethargy of $\langle u\rangle$, corresponding to energy $E_{0} e^{-\langle u\rangle}$. The difference is subtle but very significant and is due to the fact that the statistical average of a product (of energies during collisions) is not the product of the average values. Masakuni Narita and Koichi Narita ${ }^{11}$ computed the complete analytical formula for $n$ for nuclides with

[^69]
(Courtesy Pazsit)
${ }^{11}$ In Masakuni Narita, Koïchi Narita: Average number of collisions necessary for slowing down of neutrons, Journal of Nuclear Science and Technology, Vol. 26 No 9, pp819-825 (1989).
mass $>1$ using a symbolic calculator. From the very complicated expressions, they derived an approximation given by:
$$
\langle n(u)\rangle \approx C+\frac{u}{\xi}
$$

With $C=1$ for hydrogen $(A=1), C=0.8$ for deuterium $(A=2)$ and $C \approx 0.7$ for $A>2$.

### 4.2.3 Effect of the Motion of the Target Nucleus

During the slowing-down process, we have seen that the motion of the target nucleus is assumed to be negligible. However, when the velocity of the neutron decreases, the Brownian motion due to thermal agitation cannot be disregarded (for solids the motion is not pure Brownian motion). In the chapter on "Thermalization" below, we shall examine the consequences of taking this phenomenon into account. Here, the influence of this motion on the gain in lethargy will be analyzed. Like the average cosine of the scattering angle in elastic scattering $\left(\overline{\mu_{0}}\right)$, discussed in the chapter "Interactions of neutrons with matter", the gain in lethargy is averaged over all the possible scattering angles in the center of mass using the standard notations: $\mu_{0}=\cos \psi$ and $p\left(\mu_{0}\right) d \mu_{0}$ is the probability of a collision angle $\psi$ in the center of mass:

$$
\langle\xi\rangle=\frac{1}{2} \int_{-1}^{+1} \ln \left(\frac{E_{0}}{E_{1}}\right) p\left(\mu_{0}\right) d \mu_{0}=\frac{1}{2} \int_{-1}^{+1} \ln \left(\frac{E_{0}}{E_{1}}\right)\left(1+3 \overline{\mu_{0}} \mu_{0}\right) d \mu_{0} \approx \frac{1}{2} \int_{-1}^{+1} \ln \left(\frac{E_{0}}{E_{1}}\right) d \mu_{0}
$$

The approximation is obtained by assuming that the collision is reasonably isotropic in the center of mass. Using a vector diagram for velocities:

$$
\left\{\begin{array}{l}
\vec{v}_{0}=\vec{v}_{G}+\vec{v}_{0, \otimes} \\
\vec{v}_{1}=\vec{v}_{G}+\vec{v}_{1, \otimes}
\end{array} \quad \text { hence : } \quad v_{1}^{2}=v_{G}^{2}+v_{1, \otimes}^{2}+2 v_{G}^{2} v_{1, \otimes}^{2} \mu_{0}\right.
$$

$\bar{V}$ is denoted as the average velocity of the target nuclei and the ratio of the incident velocities $b \equiv v_{0} / \bar{V}$ is introduced. The laws of elastic collisions enable calculation of the velocities $v_{G}$ and $v_{1, \otimes}$ after a collision as a function of the ratio of masses $A$ and the angle between the neutron velocity and that of the nucleus in the laboratory frame, given by its cosine $\mu=\cos \varphi$ :

$$
v_{G}=\frac{\bar{V}}{A+1} \sqrt{b^{2}+A^{2}+2 b A \cos \varphi} \quad \text { and } \quad v_{1, \otimes}=\frac{A \bar{V}}{A+1} \sqrt{b^{2}+1-2 b \cos \varphi}
$$

Using:

$$
\left\{\begin{array}{l}
S \equiv \frac{v_{G}^{2}}{\bar{V}^{2}}+\frac{v_{1, \otimes}^{2}}{\bar{V}^{2}}=\frac{b^{2}+A^{2}+2 b A \cos \varphi+A^{2}\left(b^{2}+1-2 b \cos \varphi\right)}{(A+1)^{2}} \\
P \equiv 2 \frac{v_{G} v_{1, \otimes}}{\bar{V}^{2}}=2 \frac{A \sqrt{\left(b^{2}+A^{2}+2 b A \cos \varphi\right)\left(b^{2}+1-2 b \cos \varphi\right)}}{(A+1)^{2}}
\end{array}\right.
$$

The integral $\langle\xi\rangle$ can be computed analytically by substituting $\ln \left(\frac{E_{0}}{E_{1}}\right)=2 \ln \frac{v_{0}}{v_{1}}$, thus:

$$
\begin{aligned}
\langle\xi\rangle & =\frac{1}{2} \int_{-1}^{+1}\left[\ln b^{2}-\ln \left(S+P \mu_{0}\right)\right] d \mu_{0} \\
& =1+\ln b^{2}-\frac{(S+P) \ln (S+P)-(S-P) \ln (S-P)}{2 P}
\end{aligned}
$$

This expression depends on $\mu=\cos \varphi$ via the terms $S$ and $P$. The average of $\langle\xi\rangle$ over all the incident angles may be computed by assuming that the random motion of the target nuclei leads to an isotropic collision, giving:

$$
\overline{\langle\xi\rangle}=\frac{1}{2} \int_{-1}^{+1}\langle\xi\rangle d \mu=1+\ln b^{2}-\int_{-1}^{+1} \frac{(S+P) \ln (S+P)-(S-P) \ln (S-P)}{4 P} d \mu
$$

R.L. Murray performed a numerical analysis ${ }^{12}$ of this non-analytical integral in terms of $A$ and $b$ using a Gauss quadrature, and he showed that for high values of $b$, the usual expression is obtained:

$$
\xi=1-\frac{\alpha}{1-\alpha} \ln \frac{1}{\alpha}
$$

whereas for weak values, $\overline{\langle\xi\rangle}$ can be approximated by:

$$
\xi \approx 1+2 \ln \frac{b(A+1)}{2 A}
$$

### 4.2.4 Transfer Probability as a Function of Angle

We shall try to compute the probability $P\left(\vec{\Omega} \rightarrow \overrightarrow{\Omega^{\prime}}, u \rightarrow u^{\prime}\right)$ of a neutron being scattered from one direction, $\vec{\Omega}$, to another, $\overrightarrow{\Omega^{\prime}}$, by changing lethargy from $u$ to

[^70]Fig. 4.7 Collision parameters

$u^{\prime}>u$. The scattering is assumed to be isotropic in the center-of-mass frame, implying that the probability of scattering at a given angle will no longer depend on that angle but rather on the solid angle. The scattering probability density is thus $1 /(4 \pi)$. By definition, a differential element of solid angle is (Fig. 4.7):

$$
\frac{d \Omega}{4 \pi}=\frac{1}{4 \pi} \sin \psi d \psi d \theta
$$

where $\theta$ is the polar angle (co-latitude) and $\psi$ the azimuthal angle. $\theta_{0}$ is the deviation angle resulting from scattering. Deriving Eq. 4.4:

$$
\sin \psi d \psi=\frac{(A+1)^{2}}{8 \pi A} e^{-\left(u^{\prime}-u\right)} d u
$$

This equation leads to expression of the probability density of isotropic scattering towards lethargy $u^{\prime}$. Further, in the collision equations, the scattering angle in the laboratory frame is given by the following equation:

$$
\begin{equation*}
\vec{\Omega} \cdot \overrightarrow{\Omega^{\prime}}=\cos \theta_{0}=\frac{A+1}{2} \frac{v_{1}}{v_{0}}-\frac{A-1}{2} \frac{v_{0}}{v_{1}}=\frac{A+1}{2} e^{-\frac{\left(u^{\prime}-u\right)}{2}}-\frac{A-1}{2} e^{+\frac{\left(u^{\prime}-u\right)}{2}} \tag{4.11}
\end{equation*}
$$

Knowing angles $\theta, \theta^{\prime}, \psi$ and $\psi^{\prime}$ is sufficient to determine the scattering angle $\theta_{0}$, given by:

$$
\cos \theta_{0}=\cos \theta \cos \theta^{\prime}+\sin \theta \sin \theta^{\prime} \cos \left(\psi-\psi^{\prime}\right)
$$

Angle $\theta_{0}$ is the only possible angle once all the collision parameters are imposed. Therefore, the isotropic scattering probability, which depends solely on $\vec{\Omega} \cdot \overrightarrow{\Omega^{\prime}}$ $=\cos \theta_{0}$ in angular terms, and on the difference in lethargy, is obtained by:

$$
\begin{aligned}
P\left(\vec{\Omega} \rightarrow \overrightarrow{\Omega^{\prime}}, u \rightarrow u^{\prime}\right) & =P\left(\vec{\Omega} \cdot \overrightarrow{\Omega^{\prime}}, u \rightarrow u^{\prime}\right) \\
& =\frac{(A+1)^{2}}{8 \pi A} e^{-\left(u^{\prime}-u\right)} \delta\left(\cos \theta_{0}-\frac{A+1}{2} e^{-\frac{\left(u^{\prime}-u\right)}{2}}-\frac{A-1}{2} e^{+\frac{\left(u^{\prime}-u\right)}{2}}\right)
\end{aligned}
$$

using the Dirac $\delta$ function. The integral of this distribution over $4 \pi$ steradians is equal to 1 . If multiplied by a total scattering cross section, this probability leads to the differential scattering cross section $\sigma_{s}\left(\vec{\Omega} \cdot \overrightarrow{\Omega^{\prime}}, u \rightarrow u^{\prime}\right)$. The expression may be rendered more general by considering anisotropic collisions in the center of mass. Classically, the differential cross section is expanded over a Legendre polynomial expansion for the cosine of the scattering angle in the center of mass, $\mu=\cos \Psi=\vec{\Omega} \cdot \overrightarrow{\Omega^{\prime}}$ (expansion is generally truncated at order 5, even for highly anisotropic materials):

$$
\sigma_{s}\left(\mu, E \rightarrow E^{\prime}\right)=\frac{4 \pi}{(1-\alpha) E} \sum_{l=1}^{5} B_{l}(E) P_{l}(\mu)
$$

Also, from the laws of elastic collision, $\mu=1-2\left(1-E^{\prime} / E\right) /(1-\alpha)$, meaning that with this model, the differential cross section is an algebraic expression depending solely on the considered isotope and on $\mu$. In a multigroup representation in which the energy interval is divided into $n$ energy groups with upper and lower limits $\left[E_{i}, E_{i-1}\right.$ ] whose index increases as energy decreases (a universally adopted convention), the transfer cross section from energy $E$ to group $i$ is written as:

$$
\sigma_{s}\left(E \rightarrow\left[E_{i-1}, E_{i}\right]\right)=\int_{E_{i}}^{E_{i-1}} \sigma_{s}\left(E \rightarrow E^{\prime}\right) d E^{\prime}
$$

Furthermore, the transfer cross section from group $j$ to group $i$ is computed as:

$$
\sigma_{s}\left(\left[E_{j-1}, E_{j}\right] \rightarrow\left[E_{i-1}, E_{i}\right]\right)=\sigma_{s}^{j \rightarrow i}=\int_{E_{j}}^{E_{j-1}} d E \int_{E_{i}}^{E_{i-1}} \sigma_{s}\left(E \rightarrow E^{\prime}\right) d E^{\prime}
$$

which is approximated by $\frac{1}{2}\left(\sigma_{s}\left(E_{j} \rightarrow\left[E_{i-1}, E_{i}\right]\right)+\sigma_{s}\left(E_{j-1} \rightarrow\left[E_{i-1}, E_{i}\right]\right)\right)$.
In the neutron scattering equations discussed later, the transfer cross section to lower groups (or to the same group) is considered:

$$
\sigma_{r}^{j}=\sum_{i=j+1}^{i=n-1} \sigma_{s}\left(\left[E_{j-1}, E_{j}\right] \rightarrow\left[E_{i-1}, E_{i}\right]\right)+\underbrace{\sigma_{s}\left(\left[E_{j-1}, E_{j}\right] \rightarrow\left[E_{j-1}, E_{j}\right]\right.}_{\sigma_{s, 0}})
$$

### 4.2.5 Isotropic Collision

We saw earlier that the cosine of scattering angle $\theta$ in the center-of-mass frame is:

$$
\left\{\begin{array}{c}
\mu_{0} \equiv \cos \theta=\left(\frac{A}{A+1} \cos \psi+\frac{1}{A+1}\right) \frac{v_{0}}{v_{1}} \\
\left(\frac{v_{0}}{v_{1}}\right)^{2}=\frac{(A+1)^{2}}{A^{2}+2 A \cos \psi+1}
\end{array}\right.
$$

where:

$$
\mu_{0} \equiv \cos \theta=\frac{A \cos \psi+1}{\sqrt{A^{2}+2 A \cos \psi+1}}=\frac{A \mu+1}{\sqrt{A^{2}+2 A \mu+1}}
$$

with $\mu \equiv \cos \psi$ the cosine of the collision angle in the center-of-mass frame. Deriving the square of this expression, the following equation is obtained:

$$
d \mu_{0}=\left(\frac{A}{\sqrt{A^{2}+2 A \mu+1}}-\frac{1}{2} \frac{A \mu+1}{\left(A^{2}+2 A \mu+1\right)^{\frac{3}{2}}}(2 A)\right) d \mu
$$

In the case of hydrogen, where $A=1$ :

$$
d \mu_{0}=\left(\frac{1}{2 \sqrt{2+2 \mu}}\right) d \mu \quad \text { and } \quad \mu_{0}=\frac{\mu+1}{\sqrt{2 \mu+2}}=\frac{\sqrt{2} \sqrt{\mu+1}}{2}
$$

giving

$$
d \mu_{0}=\left(\frac{1}{2 \sqrt{2+2 \mu}}\right) d \mu=\frac{1}{4 \mu_{0}} d \mu
$$

Assuming that the collision is isotropic in the center of mass, the probability density, which is constant over the interval $[-1,+1]$, may be computed, and its integral is equal to 1 (by definition), i.e.:

$$
P(\mu)=\frac{1}{2}
$$

For a collision with hydrogen, the probability of reaching $\mu_{0}$ at $d \mu_{0}$ close is given by:

$$
P\left(\mu_{0}\right) d \mu_{0}=P(\mu) d \mu=\frac{1}{2} d \mu=2 \mu_{0} d \mu_{0}
$$

but only where $\mu_{0} \geq 0$, since collision with hydrogen always scatters the neutron in a forward direction.

Finally:

$$
P\left(\mu_{0}\right) d \mu_{0}= \begin{cases}2 \mu_{0} d \mu_{0} & \text { for } \mu_{0} \geq 0 \\ 0 & \text { for } \mu_{0}<0\end{cases}
$$

### 4.3 Continuous Slowing-Down Theory

(Meghreblian and Holmes 1960, p85)
If a neutron balance is carried out at energy $E$ (resp. lethargy $u$ ), fission neutrons are created at energy $E$ (respectively $u$ ), if this energy allows (hence, fast energy), with a source $S(E)$ (resp. $S(u)$ ) (Fig. 4.8).

Neutrons can also reach this energy by slowing down from a higher energy, $E^{\prime}$, through scattering on moderator nuclei. This slowing down is represented by the differential reaction rate $\Sigma_{s}\left(E^{\prime}\right) \Phi\left(E^{\prime}\right) P\left(E^{\prime} \rightarrow E\right)$ where $R_{s}\left(E^{\prime}\right)=\Sigma_{s}\left(E^{\prime}\right) \Phi\left(E^{\prime}\right)$ is the number of neutrons scattering from energy $E^{\prime}$ and $P\left(E^{\prime} \rightarrow E\right)$ is the probability of reaching $E$ by scattering from $E^{\prime}$. All scattering at higher energies than $E$ must be considered, i.e.:

Fig. 4.8 Slowing-down balance


$$
\int_{E}^{+\infty} \Sigma_{s}\left(E^{\prime}\right) \Phi\left(E^{\prime}\right) P\left(E^{\prime} \rightarrow E\right) d E^{\prime}
$$

In practice, the upper limit $+\infty$ of the integral is the maximum energy of the fast spectrum $E_{0} \approx 10 \mathrm{MeV}$. Neutrons are removed from energy $E$ through scattering and absorption, and hence through the reaction rate ${ }^{13} R_{T}(E)=\Sigma_{t}(E) \Phi(E)$. The balance is finally written as (Dresner 1960, p8):

Balance of slowing-down in energy:

$$
\begin{equation*}
\int_{E}^{+\infty} \Sigma_{s}\left(E^{\prime}\right) \Phi\left(E^{\prime}\right) P\left(E^{\prime} \rightarrow E\right) d E^{\prime}+S(E)=\Sigma_{t}(E) \Phi(E) \tag{4.12}
\end{equation*}
$$

This balance may be written in the form of lethargy:

$$
\int_{-\infty}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}+S(u)=\Sigma_{t}(u) \Phi(u)
$$

The number of neutrons undergoing a collision in the interval $[u, u+d u]$, i.e. $R_{t}(u)=\Sigma_{t}(u) \Phi(u)$, is equal to the number of neutrons set directly at this energy by the fission source $S(u)$, along with the neutrons reaching this lethargy after scattering from a lower lethargy:

$$
\int_{-\infty}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}
$$

If $u^{\prime}>u, P\left(u^{\prime} \rightarrow u\right)=0$, in mathematical terms, a neutron at lethargy $u^{\prime}$ cannot be slowed down to a lower lethargy, at least during the slowing-down phase (this is not the case for thermalization, where a neutron may gain energy).

Let $q(E)$ be the slowing-down density or slowing-down current, that is, the number of neutrons per unit time and volume scattering from above a higher energy $E$ to a lower energy. It is assumed for the moment that neutrons cannot gain energy (Fig. 4.9).

Using $q(u)$, the number of neutrons crossing the lethargy $u$ by slowing down above or beyond $u$ is expressed by the double integral:

[^71]Fig. 4.9 Slowing-down density $q(E)$


Slowing-down density : $q(u)=\int_{-\infty}^{u} \Sigma_{S}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}$

Deriving $q(u)$, the following expression is obtained ${ }^{14}$ :

$$
\begin{gathered}
\frac{d q(u)}{d u}=\Sigma_{S}(u) \Phi(u)+\left(\int_{-\infty}^{u} \frac{d}{d u} \Sigma_{S}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}\right) \\
=\Sigma_{S}(u) \Phi(u)-\underbrace{\int_{-\infty}^{u} \Sigma_{S}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} P\left(u^{\prime} \rightarrow u\right)}_{\Sigma_{t}(u) \Phi(u)-S(u)}
\end{gathered}
$$

Since $\Sigma_{t}(u)=\Sigma_{s}(u)+\Sigma_{a}(u)$, the differential equation for slowing-down is obtained using the neutron balance:

$$
\frac{d q(u)}{d u}=S(u)-\Sigma_{a}(u) \Phi(u)
$$

In the case of a monatomic, elastic and isotropic collision:

$$
P\left(u^{\prime} \rightarrow u^{\prime \prime} \leq u^{\prime}+\varepsilon\right)=P\left(u^{\prime \prime}-u^{\prime}\right)=\frac{1}{1-\alpha} e^{-\left(u^{\prime \prime}-u^{\prime}\right)} \text { and } P\left(u^{\prime} \rightarrow u^{\prime \prime}>u^{\prime}+\varepsilon\right)=0
$$

The second equation indicates that it is not possible for a neutron to acquire more than the maximum gain in lethargy $\varepsilon$. Thus, the number of neutrons transferred from lethargy $u^{\prime}$ beyond lethargy $u$ (the term crossing probability will be used) can be calculated using $e^{-\varepsilon}=\alpha$ :

$$
{ }^{14} \frac{d}{d u}\left(\int_{-\infty}^{u} f(u, v) d v\right)=f(u, u)+\int_{-\infty}^{u} \frac{d f(u, v)}{d u} d v
$$

$$
\underbrace{\int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime} \geq u\right) d u^{\prime \prime}} \quad=\int_{u}^{u^{\prime}+\varepsilon} \frac{1}{1-\alpha} e^{-\left(u^{\prime \prime}-u^{\prime}\right)} d u^{\prime \prime}=\frac{e^{-\left(u-u^{\prime}\right)}-\alpha}{1-\alpha}
$$

Number of neutrons transferred

> beyond u for a neutron
undergoing a collision at $u^{\prime}\left(u^{\prime}<u\right)$
for $0 \leq u-u^{\prime} \leq \varepsilon$; otherwise $=0$.
For a simple monatomic, elastic, isotropic and non-absorbing ( $\Sigma_{a}=0$ ) medium, the slowing-down equation reduces to:

$$
\frac{d q(u)}{d u}=S(u)
$$

If the source is represented by a Dirac distribution of intensity $S$ neutrons per unit volume and time at lethargy $u_{0}$, i.e. $S(u)=S \delta\left(u_{0}\right), q(u)$ is the Heaviside step distribution (zero neutrons before the energy value of the source and $S$ neutrons per unit volume after the source since there is no absorption) (Fig. 4.10).

Assuming a source with a unit Dirac distribution and of lethargy $u_{0}=0$, the corresponding slowing-down density will be the Heaviside unit step function $\Theta(u)$. By defining the slowing-down density, the following equation is obtained:

$$
\begin{aligned}
q(u) & =\Theta(u)=\int_{-\infty}^{u} \Sigma_{S}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime} \\
& =\int_{u-\varepsilon}^{u} R_{S}\left(u^{\prime}\right) d u^{\prime} \frac{e^{-\left(u-u^{\prime}\right)}-\alpha}{1-\alpha}
\end{aligned}
$$

This expression includes a convolution with the "crossing function" Fr:

$$
\begin{cases}\operatorname{Fr}(u) \equiv \frac{e^{-u}-\alpha}{1-\alpha} & \text { for } \quad 0 \leq u \leq \varepsilon \\ \operatorname{Fr}(u) \equiv 0 & \text { otherwise }\end{cases}
$$

having the following Laplace transform:



Fig. 4.10 Slowing-down density due to a point source in a non-absorbing medium

$$
f_{r}(s)=\frac{1}{s} \frac{\alpha^{s+1}+(1-\alpha)(s+1)-1}{(1-\alpha)(s+1)}=\frac{1}{s}(1-\varpi)
$$

with $\varpi \equiv \frac{1-\alpha^{s+1}}{(1-\alpha)(s+1)}$. Hence, using the crossing function:

$$
\begin{equation*}
q(u)=\Theta(u)=\int_{-\infty}^{u} R_{S}\left(u^{\prime}\right) F r\left(u-u^{\prime}\right) d u^{\prime} \tag{4.14}
\end{equation*}
$$

The Laplace transform of the latter equation is written as:

$$
\frac{1}{s}=r_{s}(s) f_{r}(s)
$$

where:
Scattering reaction rate image for a neutron source: $\quad r_{s}(s)=\frac{1}{1-\varpi}$
If a source neutron is emitted at $u_{0}=0$, it must necessarily be scattered by collision at this very lethargy in order to be slowed down (in which case, the neutron travels through vacuum and has a constant lethargy). This implies that the scattering rate includes a Dirac delta function at the origin. Furthermore, it is seen that the constant term:
$\frac{1}{\xi}=\frac{1}{\int_{0}^{\varepsilon} \operatorname{Fr}(u) d u}=\frac{1-\alpha}{1-\alpha-\alpha \varepsilon}$ is the asymptotic solution to Eq. 4.14.
George Placzek expressed the scattering rate created by a unit source at lethargy 0 in the following form (Dresner 1960, p9):

$$
\begin{equation*}
\Sigma_{s}(u) \Phi(u)=\delta(u)+R_{s}(u)=\delta(u)+\frac{1}{\xi}(1+\Phi(u)) \tag{4.16}
\end{equation*}
$$

This rate has a singular term, $\delta(u)$, in the sense that the source itself is singular in lethargy. $R_{s}(u)$ is the non-singular part of the scattering rate, also called the Placzek function. The function $\Phi(u)$-which in fact is not a flux-decays quickly and can be easily computed using its Laplace transform $\varphi(s)$ (Photo 4.3):

$$
\mathrm{R}_{s}(s)=1+r_{s}(s)=1+\frac{1}{\xi}\left(\frac{1}{s}+\varphi(s)\right)
$$



Photo 4.3 Georges Placzek (1905-1955) was a Russian physicist of Czech origin. After his studies in Prague, then Vienna, he worked on fission. He migrated to Denmark in 1932, and was later a professor at the University of Jerusalem and the University of Kharkov (USSR). He devised a pioneering theory on the Raman effect. After his migration to Canada, he contributed as a theorist to the Manhattan Project aspart of the British Chalk River group. From 1948, he worked at Princeton University. He died prematurely at the age of 50 (Public domain)

Hence, the image expression is:

$$
\varphi(s)=\frac{1}{s}(1-\xi) \frac{(1+\xi s)\left(1-e^{-\varepsilon s}\right)-\varepsilon s}{\varepsilon s-(1-\xi)\left(1-e^{-\varepsilon s}\right)}
$$

which is usually expanded in a series in terms of $s$ :

$$
\varphi(s)=\sum_{n=0}^{\infty} \varphi_{n} s^{n}=1-\xi-\frac{(1-\xi)}{2 \xi} \varepsilon+\left[\frac{(1-\xi)}{2 \xi} \varepsilon+\frac{3+\xi^{2}-4 \xi}{12 \xi^{2}} \varepsilon^{2}\right] s^{2}+\ldots
$$

This expansion shows the importance of integer multiples of $\varepsilon$, which will be analyzed for the slowing-down process on a target heavier than hydrogen. Comparing with Eq. 4.10, it can be seen that:

$$
\bar{n}(s)=\frac{1}{s} \frac{1}{(1-\varpi)}=\frac{1}{s} \mathrm{R}_{s}(s)
$$

Therefore, by an inverse transformation process:

$$
\overline{n(u)}=\int_{0}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime}=\int_{0}^{u}\left[\delta\left(u^{\prime}\right)+\frac{1}{\xi}\left(1+\Phi\left(u^{\prime}\right)\right)\right] d u^{\prime}=1+\frac{u}{\xi}+\frac{\Phi_{0}}{\xi}
$$

Where $\Phi_{0}=\int_{0}^{u} \Phi\left(u^{\prime}\right) d u^{\prime}=\int_{0}^{+\infty} \Phi\left(u^{\prime}\right) d u^{\prime}=1-\xi-\frac{(1-\xi)}{2 \xi} \varepsilon \quad$ is the first moment of the Placzek complementary function.

Fig. 4.11 Number of neutrons reaching energy $E$ after scattering from $E_{0}$ on non-absorbing hydrogen



### 4.3.1 Slowing Down by Non-Absorbing Hydrogen

(Ferziger and Zweifel 1966, p65)
In a seminal article, ${ }^{15}$ Amaldi and Fermi analyzed the resulting flux during slowing down by non-absorbing hydrogen. The probability of a neutron reaching energy $E$ (resp. lethargy $u$ ) following a collision immediately after its birth at energy $E_{0}$ (resp. $u_{0}=0$ ) is plotted in Fig. 4.11. In the case of hydrogen, it may be observed that any lower energy may be attained (even the theoretical value of 0 eV ) since $\alpha_{1} H=0$ at first order. This hypothesis is valid if the neutron mass is assumed to be equal to that of the hydrogen proton, which is not strictly true. The probability of energy loss $P\left(E_{0} \rightarrow E \leq E_{0}\right)$ is constant:

$$
P\left(E_{0} \rightarrow E \leq E_{0}\right)=\frac{C}{E_{0}}
$$

In terms of lethargy, this probability is expressed as:

$$
P\left(u_{0}=0 \rightarrow u\right)=C e^{-u}
$$

$C$ is a normalization constant equal to 1 if it is assumed that the neutron can be slowed down until it has no energy. In reality, the neutron gains the average energy of the slowing-down medium, thus $C$ is slightly above 1 . The differential elastic scattering cross section of hydrogen $(A=1)$ can be modeled by expanding the cosine of the scattering angle in the laboratory frame on a Legendre polynomial basis:

[^72]$$
\Sigma_{s}\left(u^{\prime} \rightarrow u, \mu_{0}\right)=\frac{1}{2} \sum_{l=0}^{+\infty}(2 l+1) \quad \Sigma_{s, l}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u, \mu_{0}\right) P_{l}\left(\mu_{0}\right)
$$
where
$\Sigma_{s, l}\left(u^{\prime} \rightarrow u\right)=\int_{-1}^{+1} \Sigma_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u, \mu_{0}\right) P_{l}\left(\mu_{0}\right) d \mu_{0}$
From Eq. 4.11, the cosine of the angle after collision depends solely on the difference of lethargies (as $A=1$ ):
$$
\mu_{0}=\frac{1}{2}\left[(A+1) e^{-\frac{u-u^{\prime}}{2}}-(A-1) e^{+\frac{u-u^{\prime}}{2}}\right]=e^{-\frac{u-u^{\prime}}{2}}
$$

After a collision at lethargy $u^{\prime}$ such that the cosine of the scattering angle is $\mu_{0}$, the probability of reaching lethargy $u$ depends solely on the change in lethargy:

$$
P\left(u^{\prime} \rightarrow u, \mu_{0}\right)=e^{-\left(u-u^{\prime}\right)} \delta\left(\mu_{0}-e^{-\frac{u-u^{\prime}}{2}}\right)
$$

The moments of the scattering cross section can thus be computed analytically:

$$
\Sigma_{s, l}\left(u^{\prime} \rightarrow u\right)=\int_{-1}^{+1} \Sigma_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u, \mu_{0}\right) P_{l}\left(\mu_{0}\right) d \mu_{0}=\Sigma_{s}\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)} P_{l}\left(e^{-\frac{u-u^{\prime}}{2}}\right)
$$

The first few moments are:

$$
\left\{\begin{array}{l}
\Sigma_{s, 0}\left(u^{\prime} \rightarrow u\right)=\Sigma_{s}\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)} \\
\Sigma_{s, 1}\left(u^{\prime} \rightarrow u\right)=\Sigma_{s}\left(u^{\prime}\right) e^{-\frac{3}{2}\left(u-u^{\prime}\right)} \\
\Sigma_{s, 2}\left(u^{\prime} \rightarrow u\right)=\Sigma_{s}\left(u^{\prime}\right) \frac{\left[3 e^{-\left(u-u^{\prime}\right)}-1\right]}{2} e^{-\left(u-u^{\prime}\right)}
\end{array}\right.
$$

For hydrogen, the collision is isotropic in the center-of-mass frame until around 9 MeV , i.e. almost the whole spectrum. The change of center-of-mass frame to the laboratory frame is taken into account in the following ( $\mu$ is the cosine of the scattering angle in the center of mass):

$$
P\left(\mu_{0}\right) d \mu_{0}=P(\mu) d \mu
$$

The isotropic collision in the center of mass leads to $P(\mu)=1 / 2$. From Eqs. 4.2 and 4.3:

$$
\begin{aligned}
\cos ^{2} \theta & =\frac{(A+1)^{2}}{4}\left(\frac{v_{1}}{v_{0}}\right)^{2}+\frac{[A-1]^{2}}{4}\left(\frac{v_{0}}{v_{1}}\right)^{2}-\frac{(A+1)(A-1)}{2} \\
& =\frac{A^{2}+1+2 A \cos \Psi}{4}+\frac{[A-1]^{2}(A+1)^{2}}{4\left(A^{2}+1+2 A \cos \Psi\right)}-\frac{(A+1)(A-1)}{2}
\end{aligned}
$$

This equation is differentiated with respect to $\mu$ and $\mu_{0}$ to obtain the probability $P(\mu)$ :

$$
2 \cos \theta d(\cos \theta)=\frac{2 A d(\cos \Psi)}{4}-\frac{[A-1]^{2}(A+1)^{2}}{4\left(A^{2}+1+2 A \cos \Psi\right)^{2}} 2 A d(\cos \Psi)
$$

or: $\mu_{0} d \mu_{0}=\left(1-\frac{[A-1]^{2}(A+1)^{2}}{\left(A^{2}+1+2 A \mu\right)^{2}}\right) \frac{A}{4} d \mu$
If applied to hydrogen, in which case the neutron is always scattered forwards ( $\mu_{0}>0$ ), the following equation can be written

$$
d \mu=\left\{\begin{array}{lll}
4 \mu_{0} d \mu_{0} & \text { if } & \mu_{0}>0 \\
0 & \text { if } & \mu_{0}<0
\end{array}\right.
$$

where: $P\left(\mu_{0}\right)=\left\{\begin{array}{lll}2 \mu_{0} & \text { if } & \mu_{0}>0 \\ 0 & \text { if } & \mu_{0}<0\end{array}\right.$
The mean cosine of the scattering angle is computed as:

$$
\overline{\mu_{0}}=\int_{-1}^{+1} \mu_{0} P\left(\mu_{0}\right) d \mu_{0}=\frac{2}{3}
$$

The higher moments of the cosine of the scattering angle characterize strong anisotropy in the laboratory frame:

$$
\overline{\mu_{0}^{2}}=\int_{-1}^{+1} \mu_{0}^{2} P\left(\mu_{0}\right) d \mu_{0}=\frac{1}{2} \quad \text { and } \quad \overline{\mu_{0}{ }^{3}}=\int_{-1}^{+1} \mu_{0}^{3} P\left(\mu_{0}\right) d \mu_{0}=\frac{2}{5}
$$

If a neutron balance is established at energy $E$, it may be assumed that some neutrons originate directly from the source of intensity $S$ by scattering after the first collision, i.e. $R_{1}\left(E_{0}\right) P\left(E_{0} \rightarrow E\right) d E=S d E / E_{0}$ (the index 1 indicates that it is the first collision directly at energy $E_{0}$, in the present case taking a normalization constant of $C=1$ ). Indeed, without absorption at $E_{0}$, all neutrons emitted by the source are scattered at a lower energy, thus $R_{1}\left(E_{0}\right)=\Sigma_{s}\left(E_{0}\right) \Phi\left(E_{0}\right)=S / E_{0}$. It is not possible for any neutrons to have energy lower than $E_{0}$ after a first collision, i.e. $R_{1}\left(E<E_{0}\right)=0$.

Other neutrons appear at energy $E$ after undergoing several previous collisions. These neutrons are referred to as $n^{\text {th }}$ collision neutrons". They are scattered in the

Fig. 4.12 Neutron balance at energy E for non-absorbing hydrogen

forward direction from energy $E^{\prime} \geq E$ to $E$ as given by the following differential rate:

$$
R_{n+1}\left(E^{\prime} \rightarrow E\right)=R_{n}\left(E^{\prime}\right) d E^{\prime} P\left(E^{\prime} \rightarrow E\right)=\frac{R_{n}\left(E^{\prime}\right) d E^{\prime}}{E^{\prime}}
$$

This formula allows computation of the scattering rate at any collision "order" by recurrence. Here, the index $n$ gives the number of collisions undergone by the neutron to reach $E^{\prime}$ from $E_{0}$. The reaction rate $R_{n}\left(E^{\prime}\right)$ itself stems from recurrence for all the possible collisions, leading to energy $E^{\prime}$ at any time. Moreover, by definition, the number of neutrons leaving energy $E$ without absorption is:

$$
\Sigma_{t}(E) \Phi(E)=\Sigma_{S}(E) \Phi(E)=R_{s}(E)
$$

It must be borne in mind that $\Phi(E)$ is the number of neutrons per $\mathrm{cm}^{2}$, per second and per unit energy (e.g. eV). For the $n^{\text {th }}$ collision neutrons scattering from $E^{\prime} \geq E$, the total number per unit energy is computed by integrating over the interval $E_{0}$ and $E$ :

$$
\int_{E}^{E^{\prime} \leq E_{0}} \frac{R_{n}\left(E^{\prime}\right) d E^{\prime}}{E^{\prime}}
$$

In the end, the neutron balance at energy $E$ is (Glasstone and Edlund 1972, p149) (Fig. 4.12):

$$
\forall E \neq E_{0} \quad \frac{S}{E_{0}} d E+d E \sum_{n=2}^{+\infty} \int_{E^{\prime}=E}^{E^{\prime}=E_{0}} \frac{R_{n}\left(E^{\prime}\right) d E^{\prime}}{E^{\prime}}=R_{s}(E) d E
$$

The first-collision term, $S / E_{0}$ has deliberately been introduced into this equation so as to show the neutron source. Nevertheless, this equation has been written only for energies lower than $E_{0}$ to avoid including the flux of unscattered neutrons $\Phi_{0}$ (neutrons which have not undergone any collisions) at that energy. At $E_{0}$, there is a singularity due to the point source. The flux at $E_{0}$ is composed of unscattered neutrons as well as scattered neutrons without any velocity change (Rayleigh scattering) in very small, though not zero, quantities due to the scattering probability law (proportional to $\left.S d E / E_{0}\right)$. Similarly, neutrons that are scattered several times but remain at $E_{0}$ must also be taken into account, even if infinitesimal in number (proportional to $\left.S\left(d E / E_{0}\right)^{n}\right)$. Asymptotically, the reaction rate is idealized as the limit of a large number of collisions, $\lim _{n \rightarrow+\infty} \sum_{m=0}^{m=n} R_{m}(E)=R_{s}(E)$, such that the integral equation is:

$$
\left\{\begin{array}{l}
\forall E<E_{0} \quad \underbrace{\frac{S}{E_{0}}}_{\begin{array}{l}
1^{\text {st }} \\
\text { term }
\end{array}}+\underbrace{\int_{E^{\prime}=E}^{E \prime \rightarrow E_{0}} \frac{R_{s}\left(E^{\prime}\right) d E^{\prime}}{E^{\prime}}}_{\begin{array}{l}
\text { multi-collision } \\
\text { term }
\end{array}}=R_{s}(E) \\
E=E_{0} \quad \\
E=E_{0} \quad \begin{array}{l}
S \times \delta\left(E-E_{0}\right)=R_{0}\left(E_{0}\right) \quad \text { corresponds to the unscattered flux } \\
\frac{S}{E_{0}}=R_{1}\left(E_{0}\right) \quad \text { corresponds to the first-collision flux }
\end{array}
\end{array}\right.
$$

The notation $E \rightarrow E_{0}$ in the integral means that the unscattered term is not taken into account. For the latter, a Dirac distribution $\delta\left(E-E_{0}\right)$ is introduced into the equation and is homogeneous (dimensionally) to the inverse of the energy, and with the following property for any continuous function $f$ :

$$
\forall E \leq E_{0}, \int_{E^{\prime}=E}^{E^{\prime}=E_{0}} f\left(E^{\prime}\right) \times \delta\left(E^{\prime}-E_{0}\right) d E^{\prime}=f\left(E_{0}\right)
$$

$R_{0}\left(E_{0}\right)$ cannot be written as $\Sigma_{s}\left(E_{0}\right) \Phi_{0}\left(E_{0}\right)$, which assumes that it is the firstcollision term. Concerning the term $R_{1}\left(E_{0}\right)=\Sigma_{s}\left(E_{0}\right) \Phi_{1}\left(E_{0}\right)$, given that there cannot be a first collision at an energy lower than $E_{0}$, it is almost completely concentrated at energy $E_{0}$. The definition of $R_{s}(E)=\Sigma_{s}(E) \Phi(E)$ here includes the unscattered term. This equation may be written in a single form, valid for any energy (Tait 1964, p68; Reuss 2003, p181):

$$
\begin{aligned}
& S \times \delta\left(E-E_{0}\right)+\int_{E^{\prime}=E}^{E \prime=E_{0}} \frac{R_{s}\left(E^{\prime}\right) d E^{\prime}}{E^{\prime}}=R_{S}(E) \quad \text { in terms of energy } \\
& S \times \delta\left(u-u_{0}\right)+\int_{u^{\prime}=u_{0}}^{u \prime=u} R_{s}\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)}=R_{s}(u) \quad \text { in terms of lethargy }
\end{aligned}
$$

Fig. 4.13 Flux spectrum of neutrons slowing down in an infinite lattice of non-absorbing hydrogen (monoenergetic source)


It may be proven that $R_{s}(E)=R_{s}^{\text {collision }}(E)+R_{s}^{\text {withoutcollision }}(E)=\frac{S}{E}+S \times \delta\left(E-E_{0}\right)$ is a solution to the integral equation. Indeed, if that solution is introduced into the integral equation, the following expression is obtained:

$$
S \times \delta\left(E-E_{0}\right)+\int_{E^{\prime}=E}^{E \prime=E_{0}} \frac{\left(\frac{S}{E^{\prime}}+S \times \delta\left(E^{\prime}-E_{0}\right)\right) d E^{\prime}}{E^{\prime}}=\frac{S}{E}+S \times \delta\left(E-E_{0}\right)
$$

This equation is verified since:

$$
\int_{E^{\prime}=E}^{E \prime=E_{0}} \frac{\left(\frac{S}{E^{\prime}}+S \times \delta\left(E^{\prime}-E_{0}\right)\right) d E^{\prime}}{E^{\prime}}=\int_{E^{\prime}=E}^{E \prime=E_{0}} \frac{S d E^{\prime}}{E^{2}}+\frac{S}{E_{0}}=\left[-\frac{1}{E^{\prime}}\right]_{E}^{E_{0}}+\frac{S}{E_{0}}=\frac{S}{E}
$$

In the end, the flux spectrum in an infinite medium filled with non-absorbing hydrogen is given by (Bekurts and Wirtz 1964, p123):

The flux spectrum in energy in an infinite medium of non-absorbing hydrogen:

$$
\begin{equation*}
\Phi(E)=\frac{S}{\Sigma_{s}(E) E}+\frac{S}{\Sigma_{s}(E)} \times \delta\left(E-E_{0}\right) \tag{4.17}
\end{equation*}
$$

The contribution of the unscattered flux is infinite since the Dirac distribution has a singular contribution at $E_{0}$. Hence, the flux tends to infinity as energy tends to 0 due to an accumulation of neutrons at 0 in the absence of absorption (Fig. 4.13).

It may reasonably be asked whether a permanent solution in a non-absorbing medium in which neutrons are continuously being injected really exists. The stationary solution may be obtained assuming that neutrons do not accumulate at any energy. In fact, the number of neutrons reaching a very low energy $\varepsilon$ close to 0 (not to be confused with the maximum gain of lethargy) is:

$$
\int_{E^{\prime}=\varepsilon}^{E \prime=E_{0}} \frac{\left(\frac{S}{E^{\prime}}+S \times \delta\left(E^{\prime}-E_{0}\right)\right) d E^{\prime}}{E^{\prime}}=\left[-\frac{1}{E^{\prime}}\right]_{\varepsilon}^{E_{0}}+\frac{S}{E_{0}}=\frac{S}{\varepsilon}
$$

This result is identical to the number of neutrons coming from their first scattering from a source $S$ placed at $\varepsilon$. Thus, the same number of neutrons must be removed to conserve a stationary solution, i.e. the source $S$ must be completely
removed by slowing-down. This result can be extended by making $\varepsilon$ tend towards 0 . The quantity $S \times \delta(E-0)=S \delta(E)$ must be deducted from zero energy, its $E=E_{0}$
integral $\int_{E=0} S \delta(E) d E$ being equal to a total source $S$, in order to obtain a stationary regime.

In terms of lethargy, the reaction rate of neutrons arriving after $n+1$ collisions at lethargy $u$ is:

$$
R_{n+1}\left(u^{\prime} \rightarrow u\right)=R_{n}\left(u^{\prime}\right) d u^{\prime} P\left(u^{\prime} \rightarrow u \leq u^{\prime}+\varepsilon\right)=R_{n}\left(u^{\prime}\right) d u^{\prime} e^{-\left(u-u^{\prime}\right)}
$$

and the neutron balance is finally expressed as:

$$
S \delta(u)+\int_{0}^{u^{\prime} \leq u} R_{s}\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)} d u^{\prime}=R_{S}(u)
$$

The trivial solution of the non-singular contribution is $R_{s}(u)=S$, which is also ${ }^{16}$ $R_{s}(E)=S / E$. The resulting flux has a singular component at the origin of lethargies and a Heaviside step function $\Theta(u)$, which indicates slowing down without neutron loss:

Flux spectrum in lethargy form for an infinite medium of non-absorbing hydrogen:

$$
\begin{equation*}
\Phi(u)=\frac{S}{\sum_{s}(u)} \Theta(u)+\frac{S}{\Sigma_{s}(u)} \times \delta(u) \tag{4.18}
\end{equation*}
$$

Since $R_{s}(E)=\Sigma_{s}(E) \Phi(E)$, the asymptotic flux spectrum is hence a hyperbolic function of the energy. The flux has a $1 / E$ shape if the scattering cross section is roughly constant, which is the case of hydrogen in water reactors (about 19 barns). This result is valid only if there is a large number of collisions, such that the limit can be computed. Thus, this remains valid for energies smaller than $\alpha E_{0}$ for a monoenergetic source at $E_{0}$, and also, for cases with a small mean gain in lethargy representing isotropic scattering (energies lower than 100 keV ). It no longer applies at higher energies due to the association of inelastic scattering and a much greater variation of the cross sections with energy. This model exhibits good agreement with the $1 / E$ shape up to 0.7 MeV when applied to carbon, the moderator used by Enrico Fermi for the first pile in Chicago. The discrepancy with the $1 / E$ law increases as the mass of the target nucleus decreases. Extending the model to light water remains acceptable.

[^73]
### 4.3.1.1 Neutronic Definition of the Napier's Constant

Let us assume a monoenergetic source with $S$ neutrons per second, at energy $E_{0}$, placed in a non-absorbing hydrogen gas. The probability of a neutron created at $E_{0}$ reaching a lower energy is:

$$
p\left(E_{0} \rightarrow E\right) d E=\frac{d E}{E_{0}}
$$

Assuming that the atomic mass of hydrogen is 1 , for a cut-off energy $E_{c}$ the slowing-down density is given by:

$$
q\left(E_{c}\right) \equiv \int_{E=E_{c}}^{E=E_{0}} \int_{E^{\prime}=0}^{E^{\prime}=E_{c}} \Sigma_{s}(E) \Phi(E) p\left(E \rightarrow E^{\prime}\right) d E^{\prime} d E
$$

This quantity is the number of neutrons crossing this cut-off energy. In a simple stationary state, the neutron density is equal to the source $S$ for any cut-off energy, since no neutrons are absorbed (non-absorbing medium). The slowing-down density for first scattering is computed as:

$$
q_{1}\left(E_{c}\right)=S \int_{E=0}^{E=E_{c}} p\left(E_{0} \rightarrow E\right) d E=S \frac{E_{c}}{E_{0}}
$$

For the density for second scattering:

$$
q_{2}\left(E_{c}\right)=\int_{E^{\prime}=E_{c}}^{E^{\prime}=E_{0}} \int_{E^{\prime \prime}=0}^{E^{\prime \prime}=E_{c}} S p\left(E_{0} \rightarrow E^{\prime}\right) p\left(E^{\prime} \rightarrow E^{\prime \prime}\right) d E^{\prime} d E^{\prime \prime}=S \frac{E_{c}}{E_{0}} \log \frac{E_{0}}{E_{c}}
$$

Then, for third scattering:

$$
\begin{aligned}
q_{3}\left(E_{c}\right) & =\int_{E^{\prime}=E_{0}}^{E^{\prime}=E_{0}} \int_{E^{\prime \prime}=E_{c}}^{E^{\prime \prime}=E^{\prime}} \int_{E^{\prime \prime \prime}=0}^{E^{\prime \prime \prime}=E_{c}} \operatorname{Sp}\left(E_{0} \rightarrow E^{\prime}\right) \times p\left(E^{\prime} \rightarrow E^{\prime \prime}\right) p\left(E^{\prime \prime} \rightarrow E^{\prime \prime \prime}\right) d E^{\prime} d E^{\prime \prime} d E^{\prime \prime \prime} \\
& =S \frac{E_{c}}{E_{0}} \int_{E^{\prime}=E_{c}}^{E^{\prime}=E_{0}} \ln \frac{E^{\prime}}{E_{c}} d E^{\prime}
\end{aligned}
$$

Using the dimensionless energy expressions $x=E^{\prime} / E_{c}$ and $x_{0}=E_{0} / E_{c}$, the following expression is obtained:

$$
q_{3}\left(E_{c}\right)=\frac{S}{x_{0}} \int_{x=1}^{x=x_{0}} \frac{\ln x}{x} d x=\frac{1}{2} \frac{S}{x_{0}} \ln ^{2} x_{0}
$$

This calculation can be extended to the slowing-down density for the $n^{\text {th }}$ scattering, which requires computation of the following integral:

$$
\int_{x=1}^{x=x_{0}} \frac{\ln ^{n-2} x}{x} d x=\frac{1}{n-1} \ln ^{n-1} x_{0}
$$

Finally, the total slowing-down density is the sum of all the partial densities for all scattering events:

$$
q\left(E_{c}\right)=\frac{S}{x_{0}}+\frac{S}{x_{0}} \frac{\ln x_{0}}{1!}+\frac{S}{x_{0}} \frac{\ln ^{2} x_{0}}{2!}+. .+\frac{S}{x_{0}} \frac{\ln ^{n} x_{0}}{n!}+. .
$$

Assuming that an infinite number of scattering events is attainable, the following series is obtained:

$$
q\left(E_{c}\right)=S=\sum_{n=0}^{n=+\infty} \frac{S}{x_{0}} \frac{\ln ^{n} x_{0}}{n!}
$$

This expression can be simplified to:

$$
x_{0}=\sum_{n=0}^{n=+\infty} \frac{\ln ^{n} x_{0}}{n!}
$$

for any value of $x_{0}>1$. If the Napier's constant $e$ is chosen, the well-known series expansion is obtained:

$$
e=\sum_{n=0}^{n=+\infty} \frac{1}{n!}
$$

It is now simple to obtain an expansion of the exponential function using $x_{0}=e^{z}$ :

$$
e^{z}=\sum_{n=0}^{n=+\infty} \frac{z^{n}}{n!}
$$

The notion of "energy attenuation with an exponential decay law" can thus be introduced as it is the attenuation of an initial source of neutrons by the constant $e$ (similar to the decay period regarding radioactivity). The number of neutrons crossing this exponential energy after $n$ scattering events in hydrogen is given by $1 /(e n!)$. Indeed, the "magical" simplicity of this result arises solely from the multiple integrations of the slowing-down density in $1 / E$. Nevertheless, this calculation gives a neutronic meaning to the Napier's constant.

### 4.3.2 Taking into Account Absorption by Hydrogen

There is no general solution if the target is now supposed to be absorbing, except in the case of hydrogen. This solution was developed by Hans Bethe (1937). The previous equations are extended by introducing a monoenergetic source of intensity $S$ :

$$
\Sigma_{t}(u) \Phi(u)=S \delta(u)+R_{t}(u)
$$

$R_{t}(u)$ is the non-singular component of the total reaction $\Sigma_{t}(u) \Phi(u)$, thus verifying the integral equation (Dresner 1960, p12):

$$
R_{t}(u)=\int_{u^{\prime}>0}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}+\Sigma_{s}(0) \Phi(0) P(0 \rightarrow u)
$$

One can see that the lower limit of the integral $u^{\prime}>0$ should not strictly set to 0 as the singular source term is treated separately. At the origin of lethargies, the total reaction rate is equal to the source since a neutron is either absorbed at that energy or scattered to higher lethargies. Thus, $S=\Sigma_{t}(0) \Phi(0)$ and the previous equation is then written as:

$$
\begin{align*}
R_{t}(u)= & \int_{0}^{u} \frac{\Sigma_{s}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} R_{t}\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)} d u^{\prime}+\frac{\Sigma_{s}(0)}{\Sigma_{t}(0)} S e^{-u} \\
& =e^{-u}\left[\int_{0}^{u} \frac{\Sigma_{s}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} R_{t}\left(u^{\prime}\right) e^{u^{\prime}} d u^{\prime}+\frac{\Sigma_{s}(0)}{\Sigma_{t}(0)} S\right] \tag{4.19}
\end{align*}
$$

Using $u=0$ in the latter equation, $R_{t}(0)=S \Sigma_{s}(0) / \Sigma_{t}(0)$. On deriving it, the following differential equation in $R_{t}(u)$ is obtained:

$$
\begin{aligned}
\frac{d R_{t}(u)}{d u} & =e^{-u} \frac{\Sigma_{s}(u)}{\Sigma_{t}(u)} R_{t}(u) e^{u}-e^{-u}\left(\int_{0}^{u} \frac{\Sigma_{s}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} R_{t}\left(u^{\prime}\right) e^{u^{\prime}} d u^{\prime}+R_{t}(0)\right) \\
& =\frac{\Sigma_{s}(u)}{\Sigma_{t}(u)} R_{t}(u)-R_{t}(u)
\end{aligned}
$$

The expression in brackets is simplified using Eq. 4.17. Introducing the absorption cross section $\Sigma_{a}(u)=\Sigma_{t}(u)-\Sigma_{s}(u)$, the following equation is obtained:

$$
\frac{d R_{t}(u)}{d u}=-\frac{\Sigma_{a}(u)}{\Sigma_{t}(u)} R_{t}(u)
$$

the solution of which is: $R_{t}(u)=S \frac{\Sigma_{s}(0)}{\Sigma_{t}(0)} e^{-\int_{0}^{u} \frac{\Sigma_{a}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} d u^{\prime}}$
The slowing-down density is given by:

$$
q(u)=\int_{0}^{u} \frac{\Sigma_{s}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} R_{t}\left(u^{\prime}\right) d u^{\prime} \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}+\frac{\Sigma_{s}(0)}{\Sigma_{t}(0)} S \int_{u}^{+\infty} P\left(0 \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}=R_{t}(u)
$$

Normalized to a unit source, $q(u)$ is simply the resonance escape probability $p$ $(u)$ at lethargy $u$, which will be introduced in the chapter on resonant absorption. It is the number of neutrons that survive until lethargy $u$ for one emitted neutron. It should be mentioned that (Dresner 1960, p13) developed the analytical solution for cases where the ratio of the scattering cross section to the total cross section is constant with lethargy.

### 4.3.3 Taking Account of a Spectral Source

In the case of hydrogen, with a general spectral source $S(u)$, the slowing-down equation in absorbing hydrogen is written as:

$$
S(u)+\int_{0}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)} d u^{\prime}=\Sigma_{t}(u) \Phi(u)
$$

Using the linear property of this equation with respect to the source (taking $\Phi_{a}$ as the solution to a problem with source $S_{a}$, and $\Phi_{b}$ as the solution to another problem with source $S_{b}, \Phi_{a}+\Phi_{b}$ is then the solution to $S_{a}+S_{b}$ ), the general solution to this equation is a convolution of the source by a Green function. The latter is given in terms of the flux spectrum $\varphi\left(u_{0} \rightarrow u\right)$ in the established stationary state in absorbing hydrogen after the introduction of a unit source $\delta\left(u-u_{0}\right)$ :

$$
\Phi(u)=\int_{u_{0}=0}^{u_{0}=+\infty} S\left(u_{0}\right) \varphi\left(u_{0} \rightarrow u\right) d u_{0}
$$

The Green function has a singular component due to the point nature of the energy source and a regular component for the contribution from multi-scattering (Reuss 2003, p186):

$$
\varphi\left(u_{0} \rightarrow u\right)=\frac{1}{\Sigma_{t}(u)} \times \delta\left(u-u_{0}\right)+\frac{1}{\Sigma_{t}(u)} \frac{\Sigma_{s}\left(u_{0}\right)}{\Sigma_{t}\left(u_{0}\right)} \Theta\left(u-u_{0}\right) e^{-\int_{u^{\prime}=u_{0}}^{u^{\prime}=u} \frac{\Sigma_{a}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} d u^{\prime}}
$$

### 4.3.4 Slowing Down by Targets Heavier Than Hydrogen

(Ferziger and Zweifel 1966, p69)
Hydrogen is a special case since the part of the energy spectrum lower than $E_{0}$ may be reached after scattering given that $\alpha_{H}=0$. Therefore, the neutron balance equation always includes a scattering term from the source energy, $S / E_{0}$. Extension to moderators heavier than hydrogen uses the target's $\alpha$ in the expressions. If there is no absorption, the number of neutrons reaching lethargy $u \neq u_{0}=0$ is equal to the scattering rate at that lethargy since there is no source for all values of $u$. Considering a lethargy that may be reached after scattering of a neutron immediately after its emission at lethargy $u_{0}$, the neutron balance equation includes a term for the first possible collision with a source neutron, but otherwise, only neutrons with $n$ scattering events may attain that lethargy. This logic is quite confusing as it consists in counting the first scattering term at the source $S P\left(u_{0} \rightarrow u\right)$ in the neutron balance for $u_{0}<u \leq u_{0}+\varepsilon$. This term could be included "naturally" in the total scattering $\operatorname{term} \int_{u_{0}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}$, hence, $\int_{u^{\prime}>u_{0}}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}$, where the lower limit of the integral $u^{\prime}>u_{0}$ means that neutrons from first-collision rate $S P\left(u_{0} \rightarrow u\right)$ are not counted. Using the asymptotic reaction rate $\Sigma_{s}(u) \Phi(u)$ is equivalent to integrating the first-collision events and avoids making a particular case for first scattering from the source itself. Besides, if $u$ tends towards $u_{0}$, neutrons that do not disappear by absorption are systematically removed by scattering at lethargy $u_{0}$ (at least in an infinite medium). Thus, the scattering density (which does not contain the non-scattering component) at $u_{0}$, must necessarily be equal to the source (Tait 1964, p70):

$$
\begin{aligned}
& \text { If } u=u_{0} \quad S=\Sigma_{s}\left(u_{0}\right) \Phi\left(u_{0}\right) \\
& \text { If } u_{0}<u \leq u_{0}+\varepsilon, \quad S P\left(u_{0} \rightarrow u\right)+\int_{u^{\prime}>u_{0}}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\Sigma_{s}(u) \Phi(u) \\
& \text { If } u>u_{0}+\varepsilon \quad \int_{u_{0}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\Sigma_{s}(u) \Phi(u)
\end{aligned}
$$

It may be seen that for higher energies, there can no longer be any term for scattering from the source itself; let us examine the consequences for the asymptotic regime. If the scattering rate $R_{s}$ is introduced, the resulting integral equation is known as the Placzek equation, named after George Placzek, since he
was the first to analyze the mathematical behavior $(1946)^{17}$ of a non-absorbing medium:

$$
\int_{-\infty}^{u} R_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=R_{s}(u)
$$

Since the probability $P\left(u^{\prime} \rightarrow u\right) d u^{\prime}$ is normalized to 1 (which may in fact be obtained by direct calculation):

$$
\int_{-\infty}^{u} P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\int_{u-\varepsilon}^{u} \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime}=1
$$

The constant reaction rate $R_{0}$ is an asymptotic, or trivial, solution to the Placzek equation. $R_{0}$ can be computed using the definition of the slowing-down density $q$ $(u)=S$ in the absence of absorption:

$$
q(u)=\int_{-\infty}^{u} \Sigma_{S}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime} \leq u^{\prime}+\varepsilon\right) d u^{\prime \prime}
$$

Since

$$
\begin{aligned}
& \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}=\int_{u}^{u^{\prime}+\varepsilon} \frac{e^{-\left(u^{\prime \prime}-u^{\prime}\right)}}{1-\alpha} d u^{\prime \prime}=\left[-\frac{e^{-\left(u^{\prime \prime}-u^{\prime}\right)}}{1-\alpha}\right]_{u}^{u^{\prime}+\varepsilon}=\frac{e^{-\left(u-u^{\prime}\right)}-\alpha}{1-\alpha}, \\
& q(u)=\int_{-\infty}^{u} R_{S}\left(u^{\prime}\right) d u^{\prime} \int_{u}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime} \leq u^{\prime}+\varepsilon\right) d u^{\prime \prime}=\int_{u-\varepsilon}^{u} R_{0} \frac{e^{-\left(u-u^{\prime}\right)}-\alpha}{1-\alpha} d u^{\prime}=R_{0} \xi=S
\end{aligned}
$$

leading to: $R_{0}=\frac{S}{\xi}=R_{s}(u)$
This result means that the $S$ neutrons produced gain on average $\xi$ lethargy units per collision. The scattering rate (density of scattered neutrons per unit time) is thus $R_{s}(u) \xi=S$, i.e.:

$$
\Phi(u)=\frac{S}{\xi \Sigma_{s}(u)} \quad \text { or, in energy terms : } \quad \Phi(E)=\frac{S}{\xi \Sigma_{s}(E) E}
$$

An asymptotic flux expression in the form of $1 / E$ is obtained, and is consistent with Fermi's expression for hydrogen since $\xi_{1}{ }_{1}=1$. Studying the integral equation:

[^74]$$
R(E)=\int_{E}^{E_{0}} \frac{R\left(E^{\prime}\right)}{E^{\prime}(1-\alpha)} d E^{\prime} \quad \text { or its lethargy form : } \quad R(u)=\int_{u-\varepsilon}^{u} \frac{R\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime}
$$
led Placzek to consider different reaction rates after $n$ scattering events $R_{n}(E)$ (resp. $\left.R_{n}(u)\right)$ which are solutions of the equation. In the case of the very first scattering of the neutron immediately after its emission at lethargy $u_{0}=0$, the number of once-collided neutrons, with energy $E_{0}$ and arriving at energy $E$ for a second collision, is given by:
$$
R_{2}(E)=R_{1}\left(E_{0}\right) p\left(E_{0} \rightarrow E\right)=\frac{S}{E_{0}(1-\alpha)} \quad \text { for } \quad \alpha E_{0} \leq E \leq E_{0}
$$
or in lethargy terms $R_{2}(u)=R_{1}(0) p(0 \rightarrow u)=S \frac{e^{-u}}{1-\alpha}$ for $0 \leq u \leq \varepsilon$
$R_{2}(E)$ is the scattering rate of neutrons undergoing a second scattering at energy $E$, after having been scattered a first time at $E_{0}$. If third scattering events are now considered, the contribution of the neutrons with first collisions at $E^{\prime}$ (resp. $u^{\prime}$ ) i.e. $R_{1}\left(E_{0}\right) p\left(E_{0} \rightarrow E^{\prime}\right) d E^{\prime}$ (resp. $\left.R_{1}(0) p\left(0 \rightarrow u^{\prime}\right) d u^{\prime}\right)$ and undergoing their second scattering, produce a third-scattering density of:
\[

\left\{$$
\begin{array}{l}
d R_{3}\left(E_{0} \rightarrow E^{\prime} \rightarrow E\right)=\frac{R_{1}\left(E_{0}\right) p\left(E_{0} \rightarrow E^{\prime}\right) d E^{\prime}}{(1-\alpha) E^{\prime}}=\frac{S d E^{\prime}}{E_{0}(1-\alpha)^{2} E^{\prime}} \text { for } \alpha E_{0} \leq E^{\prime} \leq E_{0} \\
d R_{3}\left(0 \rightarrow u^{\prime} \rightarrow u\right)=R_{1}(0) p\left(0 \rightarrow u^{\prime}\right) d u^{e^{-\left(u-u^{\prime}\right)}} \frac{e^{-(-\alpha}}{1-\alpha} \frac{e^{-u^{\prime}}}{1-\alpha} \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime}=S \frac{e^{-u}}{(1-\alpha)^{2}} d u^{\prime} \\
\text { for } 0 \leq u^{\prime} \leq \varepsilon
\end{array}
$$\right.
\]

The contribution of neutrons from first scattering is zero where $E^{\prime}<\alpha E_{0}$ (resp. $u^{\prime}>\varepsilon$ ). Similarly, it is not possible for second-scattering neutrons to reach $E<\alpha^{2}$ $E_{0}$ (resp. $u>2 \varepsilon$ ). The rate for neutrons of third scattering is computed by integration of the differential quantities:

$$
\left\{\begin{aligned}
R_{3}\left(E_{0} \rightarrow E\right) & =\int_{E^{\prime}=\alpha E_{0}}^{E^{\prime}=E_{0}} d R_{3}\left(E_{0} \rightarrow E^{\prime} \rightarrow E\right) d E^{\prime} \\
R_{3}(0 \rightarrow u) & =\int_{u^{\prime}=0}^{u^{\prime}=\varepsilon} d R_{3}\left(0 \rightarrow u^{\prime} \rightarrow u\right) d u^{\prime}
\end{aligned}\right.
$$

The contribution to the fourth scattering is thus calculated as:

$$
\left\{\begin{array}{l}
d R_{4}\left(E^{\prime} \rightarrow E\right)=\frac{R_{3}\left(E^{\prime}\right) d E^{\prime}}{(1-\alpha) E^{\prime}} \quad \text { for } \frac{E}{\alpha} \geq E^{\prime} \geq E \\
d R_{4}\left(u^{\prime} \rightarrow u\right)=R_{3}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime} \quad \text { for } u-\varepsilon \leq u^{\prime} \leq u
\end{array}\right.
$$

and so on for the higher scatterings. The differential contribution must be integrated over the lethargy interval where the first scattering density is not zero, i.e. $\left[E_{0}, \alpha E_{0}\right]$ (resp. $[0, \varepsilon]$ ), to obtain the scattering rate for the third collisions, which is not zero, on $\left[E_{0}, \alpha^{2} E_{0}\right]$ (resp. $[0,2 \varepsilon]$ in lethargy).

For $E \geq \alpha E_{0}, R_{3}(E)=\int_{E^{\prime}=E}^{E \prime=E_{0}} \frac{S d E^{\prime}}{E_{0}(1-\alpha)^{2} E^{\prime}}=\frac{S}{E_{0}(1-\alpha)^{2}} \ln \frac{E_{0}}{E}$
For $\alpha^{2} E_{0} \leq E \leq \alpha E_{0}$,

$$
\begin{aligned}
R_{3}(E) & =\int_{E^{\prime}=\alpha E_{0}}^{E \prime=\frac{E}{\alpha}} \frac{S d E^{\prime}}{E_{0}(1-\alpha)^{2} E^{\prime}}=\frac{S}{E_{0}(1-\alpha)^{2}} \ln \left(\frac{E}{\alpha^{2} E_{0}}\right) \\
& =\frac{S}{E_{0}(1-\alpha)^{2}}\left(2 \varepsilon-\ln \frac{E_{0}}{E}\right)
\end{aligned}
$$

It can be seen that $R_{3}(E)$ is a triangle with a vertex of $S \varepsilon /\left[E_{0}(1-\alpha)^{2}\right]$ if energy is expressed on a logarithmic scale. It should be carefully noted that $R_{3}(E)$, as defined by:

$$
\left\{\begin{aligned}
R_{3}(u)=\int_{u^{\prime}=0}^{u^{\prime}=u} \frac{S e^{-u} d u^{\prime}}{(1-\alpha)^{2}} & =\frac{S e^{-u}}{(1-\alpha)^{2}} u \quad \text { for } 0 \leq u \leq \varepsilon \\
R_{3}(u)=\int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=u} d R_{3}(u) & =\int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=\varepsilon} \frac{R_{1}\left(u^{\prime}\right) p\left(0 \rightarrow u^{\prime}\right) d u^{\prime}}{(1-\alpha)}+\underbrace{\int_{u^{\prime}=\varepsilon}^{u^{\prime}=u} \frac{R_{1}\left(u^{\prime}\right)}{\frac{u_{p\left(0 \rightarrow u^{\prime}\right)}^{(1-\alpha)}}{0} d u^{\prime}}}_{0} \\
& =\frac{S e^{-u}}{(1-\alpha)^{2}}(2 \varepsilon-u) \text { for } \varepsilon \leq u \leq 2 \varepsilon
\end{aligned}\right.
$$

is not a triangle if defined in terms of lethargy. The successive integrations smoothen the scattering probability density for multiple collisions. Hence, for $R_{4}(E)$, a pseudo-parabolic profile is obtained (Fig. 4.14).

$$
\begin{aligned}
R_{4}(u) & =\int_{u^{\prime}=0}^{u^{\prime}=u} \frac{S e^{-u} u^{\prime} d u^{\prime}}{(1-\alpha)^{3}}=\frac{S e^{-u}}{(1-\alpha)^{3}} \frac{u^{2}}{2} \quad \text { for } 0 \leq u \leq \varepsilon \\
R_{4}(u) & =\int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=\varepsilon} \frac{S e^{-u} u^{\prime} d u^{\prime}}{(1-\alpha)^{3}}+\int_{u^{\prime}=\varepsilon}^{u^{\prime}=u} \frac{S e^{-u}\left(2 \varepsilon-u^{\prime}\right) d u^{\prime}}{(1-\alpha)^{3}} \\
& =\frac{S e^{-u}}{(1-\alpha)^{3}}\left[\left(\frac{\varepsilon^{2}}{2}-\frac{(u-\varepsilon)^{2}}{2}\right)+2 \varepsilon(u-\varepsilon)-\frac{u^{2}}{2}+\frac{\varepsilon^{2}}{2}\right]
\end{aligned}
$$



Fig. 4.14 Constructing the probability density for second scattering and its generalization

$$
\begin{aligned}
& =\frac{S e^{-u}}{(1-\alpha)^{3}}\left[-u^{2}+3 \varepsilon u-\frac{3}{2} \varepsilon^{2}\right] \quad \text { for } \varepsilon \leq u \leq 2 \varepsilon \\
R_{4}(u) & =\int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=2 \varepsilon} \frac{S e^{-u}\left(2 \varepsilon-u^{\prime}\right) d u^{\prime}}{(1-\alpha)^{3}}=\frac{S e^{-u}}{(1-\alpha)^{3}}\left[2 \varepsilon(3 \varepsilon-u)-\frac{4 \varepsilon^{2}}{2}+\frac{(u-\varepsilon)^{2}}{2}\right] \\
& =\frac{S e^{-u}}{(1-\alpha)^{3}}\left[\frac{u^{2}}{2}-3 \varepsilon u+\frac{9}{2} \varepsilon^{2}\right] \quad \text { for } 2 \varepsilon \leq u \leq 3 \varepsilon
\end{aligned}
$$

The possible scatterings are finally obtained by summing over the different scattering terms, ideally up to infinity as defined by a Von Neumann ${ }^{18}$ series. Nevertheless, the number of possible scattering events before absorption is finite for a true absorbing medium ${ }^{19}$ :

$$
R_{s}(u)=\sum_{i=2}^{\infty} R_{i}(u)
$$

The sum starts at index 2 to avoid including the singular term $R_{1}(u)=S \delta(u)$ and to remain consistent with the definition of Eq. 4.16: $\Sigma_{s}(u) \Phi(u)=S \delta(u)+R_{s}(u)$. This scattering rate shows that there is a discontinuity at lethargy $u=\varepsilon$, a discontinuity of its first derivative at $u=2 \varepsilon$, and, by recurrence, a discontinuity of the $n^{\text {th }}$ derivative at $u=(n+1) \varepsilon$ (Dresner 1960, p11). This phenomenon is characteristic of Placzek wiggles. It should be noted that where:

$$
R_{n+1}(\varepsilon)=\frac{S \alpha}{(1-\alpha)^{n}} \frac{\varepsilon^{n-1}}{(n-1)!} \quad \text { for } n \geq 2 \quad \text { and } \quad R_{1}(\varepsilon)=0
$$

the following is obtained: $R_{S}\left(\varepsilon^{-}\right)=\frac{S \alpha}{1-\alpha} \sum_{n=1}^{\infty} \frac{\left(\frac{\varepsilon}{1-\alpha}\right)^{n-1}}{(n-1)!}=\frac{S \alpha}{1-\alpha} e^{\frac{\varepsilon}{1-\alpha}}$

[^75]

[^76]whereas:
$$
R_{s}\left(\varepsilon^{+}\right)=\frac{S \alpha}{1-\alpha}\left(e^{\frac{\varepsilon}{1-\alpha}}-1\right)
$$
since $R_{2}\left(\varepsilon^{+}\right)=0$ and $R_{2}\left(\varepsilon^{-}\right)=S \alpha /(1-\alpha)$. The difference $R_{s}\left(\varepsilon^{-}\right)-R_{s}\left(\varepsilon^{+}\right)=S \alpha /$ $(1-\alpha)$ increases as the mass of the target nucleus increases (i.e. where $\alpha \rightarrow 1$ ). This difference indicates the discontinuity in the scattering rate. For lethargies higher than $\varepsilon$, the scattering rate is always continuous. Furthermore, it verifies the following equation:
\[

$$
\begin{equation*}
R_{s}(u)=\int_{u-\varepsilon}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}+\underbrace{\Sigma_{s}(0) \Phi(0)}_{s} P(0 \rightarrow u \leq \varepsilon) \tag{4.20}
\end{equation*}
$$

\]

with: $P\left(u^{\prime} \rightarrow u\right)=\frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} \quad$ and $\quad\left\{\begin{array}{l}P(0 \rightarrow u \leq \varepsilon)=\frac{e^{-u}}{1-\alpha} \\ P(0 \rightarrow u>\varepsilon)=0\end{array}\right.$
Deriving the latter balance equation, the following is obtained with $\varepsilon=\log ^{1 / \alpha}$ and $e^{-\varepsilon}=\alpha$ :

$$
\begin{aligned}
\frac{d R_{s}(u)}{d u} & =\frac{d}{d u}\left[\frac{e^{-u}}{1-\alpha}\left(\int_{u-\varepsilon}^{u} R_{s}\left(u^{\prime}\right) e^{u^{\prime}} d u^{\prime}+S\right)\right] \\
& =\frac{e^{-u}}{1-\alpha}[\left(R_{s}(u) e^{u}-R_{S}(u-\varepsilon) e^{u-\varepsilon}\right)-\underbrace{\left(\int_{u-\varepsilon}^{u} R_{S}\left(u^{\prime}\right) e^{u^{\prime}} d u^{\prime}+S\right)}_{(1-\alpha) e^{u} R_{s}(u)}] \\
& =\frac{\alpha}{1-\alpha}\left(R_{S}(u)-R_{s}(u-\varepsilon)\right)
\end{aligned}
$$

except at $u=0$ and $u=\varepsilon$, where the term $P(0 \rightarrow u \leq \varepsilon)$ is not differentiable. The term $R_{s}(u-\varepsilon)$ does not exist if $u>\varepsilon$. In the interval, this differential equation can be integrated as:

$$
R_{S}(u)=R_{S}\left(0^{+}\right) e^{\frac{\alpha}{1-\alpha} u}=\frac{1}{1-\alpha} e^{\frac{\alpha}{1-\alpha} u}
$$

$R_{s}\left(0^{+}\right)$is obtained by making $u$ tend to 0 in Eq. 4.18.
Similarly over the interval $] \varepsilon, 2 \varepsilon[$, the differential equation can be integrated (Dresner 1960, p10) by observing that $R_{s}\left(\varepsilon^{+}\right)=\frac{\alpha}{1-\alpha}\left(e^{\frac{\varepsilon}{1-\alpha}}-1\right)$ using a limit approach on the balance equation:

$$
R_{S}(u)=\frac{1}{1-\alpha} e^{\frac{\alpha}{1-\alpha} u}\left[1-\left(1-\frac{\varepsilon-u}{1-\alpha}\right) e^{-\frac{\varepsilon}{1-\alpha}}\right]
$$

By subsequent integrations, the scattering rate is obtained for higher lethargies.
The Placzek function is defined as the product $p_{A}\left(E / E_{0}\right)=E_{0} R_{s}(E)$, given for a unit source. It is classically plotted (Fig. 4.15) in a reduced form (Dresner 1960, p10; Ferziger and Zweifel 1966, p74; Meghreblian and Holmes 1960, p98):

$$
(1-\alpha) \frac{E}{E_{0}} p_{A}\left(\frac{E}{E_{0}}\right)=(1-\alpha) R_{s}(u)=f\left(\frac{u}{\varepsilon}\right)
$$

$p_{A}\left(E / E_{0}\right)$ tends towards the asymptote $E_{0} /(\xi E)$ when $E \rightarrow 0(i . e . u \rightarrow+\infty)$, and the reduced function tends to $(1-\alpha) / \xi$.

Physically speaking, at the beginning of the slowing-down process, fission neutrons are emitted with an energy spectrum (Watt spectrum) that overwhelms Placzek wiggles, which is why this discontinuity is usually not seen in an actual reactor spectrum.

Fig. 4.15 The reduced Placzek function
$(1-\alpha) \frac{E}{E_{0}} p_{A}\left(\frac{E}{E_{0}}\right)=(1-\alpha)$ $R_{s}(u)$ Adapted from Reactor Physics Constants ANL-5800, 1963


### 4.3.5 Influence of the Fast Fission Spectrum

(GA tome 1 1967, p217; Meghreblian and Holmes 1960, p119)
Taking into account the fission spectrum, the neutron balance equation in a pure scattering medium in a stationary state is written as:

$$
S \chi(u)+\int_{u_{0}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\Sigma_{s}(u) \Phi(u)
$$

In an asymptotic case, far removed from the neutron sources (at a given energy), i.e. assuming that the lethargy limit of the fission spectrum is $u_{c} \approx 100 \mathrm{keV}$, for a minimum lethargy of $u_{c}+2 \varepsilon$, it can be said that the resulting spectrum at lethargy $u$ is the sum of the asymptotic components of the point sources $S \chi\left(u^{\prime}\right) d u^{\prime}$ placed at $u^{\prime}$ (Fig. 4.16):

The asymptotic component of the source $S \chi\left(u^{\prime}\right) d u^{\prime}$ at $u$ is given by:

$$
d R_{s}\left(u^{\prime}\right)=\frac{S \chi\left(u^{\prime}\right) d u^{\prime}}{\xi} \quad \text { or } \quad d R_{s}\left(E^{\prime}\right)=\frac{S_{\chi}\left(E^{\prime}\right) d E^{\prime}}{\xi E}
$$

The resulting equation is obtained by integrating over the whole energy spectrum:

$$
R_{s}(u)=\int_{0}^{u_{c}} d R_{s}\left(u^{\prime}\right)=\frac{S}{\xi} \int_{0}^{u_{c}} \chi\left(u^{\prime}\right) d u^{\prime}
$$

or, expressed in energy terms:


Fig. 4.16 Collision density due to a fission spectrum

$$
R_{s}(E)=\int_{E_{c}}^{E_{0}} d R_{s}\left(E^{\prime}\right)=\frac{S}{\xi E} \int_{E_{c}}^{E_{0}} \chi\left(E^{\prime}\right) d E^{\prime}
$$

Note that: $\quad \chi(E) d E=\chi(E) E d u \approx \frac{2}{\sqrt{\pi}} \sqrt{0.775 E_{0} e^{-u}} e^{-0,775 E_{0} e^{-u}} 0.775 E_{0} e^{-u}$ $d u=\chi(u) d u$

This asymptotic result has physical meaning only for lethargies that correspond to energy values below 100 keV where there are no fission neutrons. Analytical formulae such as the Leachman formula (1955), $\chi(E) \equiv \frac{2}{\sqrt{\pi}} 0.775 \sqrt{0.775 E} e^{-0.775 E}$, are normalized to 1 by construction:

$$
\int_{0}^{\infty} \chi(E) d E=\frac{2}{\sqrt{\pi}} \int_{0}^{\infty} \sqrt{0.775 E} e^{-0.775 E} 0.775 d E=\frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}\right)=1
$$

or else a similar Watt spectrum enables the analytical calculation to be performed by writing the spectrum in canonical form:

$$
\chi(E)=\frac{2}{\sqrt{\pi} T^{\frac{3}{2}}} \sqrt{E e}-\text { with } T=\frac{1}{0.775}=1.29 \mathrm{MeV}^{-1}
$$

As discussed earlier, the fission spectrum can be integrated analytically using the error function:

$$
\begin{aligned}
& \operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^{2}} d t=\frac{2}{\sqrt{\pi}} \int_{0}^{x^{2}} \frac{1}{2 \sqrt{t}} e^{-t} d t \\
& \int_{E_{i}}^{E_{f}} \chi(E) d E=\frac{2}{\sqrt{\pi}}\left(\sqrt{\frac{E_{i}}{T}} e^{-\frac{E_{i}}{T}}-\sqrt{\frac{E_{f}}{T}} e^{-\frac{E_{f}}{T}}\right)+\operatorname{erf}\left(\sqrt{\frac{E_{f}}{T}}\right)-\operatorname{erf}\left(\sqrt{\frac{E_{i}}{T}}\right)
\end{aligned}
$$

Finally, the scattering rate is written as:

$$
R_{s}(E)=\frac{S}{\xi E}\left(\frac{2}{\sqrt{\pi}}\left(\sqrt{\frac{E_{c}}{T}} e^{-\frac{E_{i}}{T}}-\sqrt{\frac{E_{0}}{T}} e^{-\frac{E_{f}}{T}}\right)+\operatorname{erf}\left(\sqrt{\frac{E_{0}}{T}}\right)-\operatorname{erf}\left(\sqrt{\frac{E_{c}}{T}}\right)\right)
$$

Let us consider a situation corresponding to an energy at which neutrons are directly emitted by fission (i.e. $E>100 \mathrm{keV}$ ). This situation is not a perfectly established asymptotic case. The neutron balance is written as:

$$
\left\{\begin{array}{ll}
S \chi(u)+\int_{u_{0}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\Sigma_{s}(u) \Phi(u) & \text { pour }
\end{array} \quad u \leq u_{0}+\varepsilon .\right.
$$

The only difference is on the lower limit of the integral, which is fixed $\left(=u_{0}\right)$ for the case $u \leq u_{0}+\varepsilon$. Deriving the neutron balance wrt.u, we get the following equation:

$$
\left\{\begin{array}{l}
\frac{d R_{s}(u)}{d u}=\frac{d\left(\Sigma_{s}(u) \Phi(u)\right)}{d u}=S \frac{d \chi(u)}{d u}+R_{s}(u) \underbrace{P(u \rightarrow u)}_{1 /(1-\alpha)} \text { pour } u \leq u_{0}+\varepsilon \\
\frac{d R_{s}(u)}{d u}=\frac{d\left(\Sigma_{s}(u) \Phi(u)\right)}{d u}=S \frac{d \chi(u)}{d u}+R_{s}(u) \underbrace{P(u \rightarrow u)}_{1 /(1-\alpha)}-R_{s}(u-\varepsilon) \underbrace{P(u-\varepsilon \rightarrow u)}_{\alpha /(1-\alpha)} \text { pour } u \geq u_{0}+\varepsilon .
\end{array}\right.
$$

For the first equation $\left(u \leq u_{0}+\varepsilon\right)$, the solution of the homogeneous equation is $R_{s}(u)=C e^{\frac{u}{1-\alpha}} . C$ can be deduced by the traditional variation method:

$$
\frac{d R_{s}(u)}{d u}=C(u) \frac{1}{1-\alpha} e^{\frac{u}{1-\alpha}}+\frac{d C(u)}{d u} e^{\frac{u}{1-\alpha}}=S \frac{d \chi(u)}{d u}+\frac{C(u) e^{\frac{u}{1-\alpha}}}{1-\alpha}
$$

that is: $\frac{d C(u)}{d u}=S \frac{d \chi(u)}{d u} e^{-\frac{u}{1-\alpha}}$

$$
\begin{aligned}
C(u) & =\int_{0}^{u} S \frac{d \chi\left(u^{\prime}\right)}{d u^{\prime}} e^{-\frac{u^{\prime}}{1-\alpha}} d u^{\prime}=S\left[\chi\left(u^{\prime}\right) e^{-\frac{u^{\prime}}{1-\alpha}}\right]_{0}^{u}+\int_{0}^{u} \frac{S}{1-\alpha} \chi\left(u^{\prime}\right) e^{-\frac{u^{\prime}}{1-\alpha}} d u^{\prime} \\
& =S \chi(u) e^{-\frac{u}{1-\alpha}}+\int_{0}^{u} \frac{S}{1-\alpha} \chi\left(u^{\prime}\right) e^{-\frac{u^{\prime}}{1-\alpha}} d u^{\prime}
\end{aligned}
$$

Finally: $R_{S}(u)=S \chi(u)+e^{\frac{u}{1-\alpha}} \int_{0}^{u} \frac{S}{1-\alpha} \chi\left(u^{\prime}\right) e^{-\frac{u^{\prime}}{1-\alpha}} d u^{\prime}$ for $u \leq u_{0}+\varepsilon$
The second equation $\left(u \geq u_{0}+\varepsilon\right)$ must be considered numerically for each case, and particularly where $\varepsilon$ is very small compared to 1 (heavy moderator). In the latter event, it may reasonably be assumed that $R_{s}(u-\varepsilon) \approx R_{s}(u)$, leading to:

$$
\frac{d R_{s}(u)}{d u}=S \frac{d \chi(u)}{d u}+R_{s}(u)
$$

the solution of which is:

$$
R_{S}(u)=S \chi(u)+e^{u} \int_{0}^{u} S \chi\left(u^{\prime}\right) e^{-u^{\prime}} d u^{\prime} \text { for } u \leq u_{0}+\varepsilon \text { and where } \varepsilon \text { is very low. }
$$

These solutions are pseudo-asymptotic, established for weak lethargy values, and are not exact from a theoretical point of view because the Placzek wiggles are not present. For an exact solution, numerical integration is carried out using spectral bands.

### 4.3.6 Mixture of Moderators

(Dresner 1960, p20; Ferziger and Zweifel 1966, p78)
Supposing that the scattering medium consists of several target nuclei of moderating power $\xi_{i}$ and scattering parameter $\alpha_{i}$, the scattering density resulting from the partial scattering densities can be written as (Stacey 2001, p97):

$$
R_{s}(E)=\sum_{i \in \text { moderators }} \int_{E}^{\frac{E}{\alpha_{i}}} \frac{R_{s i}\left(E^{\prime}\right) d E^{\prime}}{E^{\prime}\left(1-\alpha_{i}\right)}
$$

Since the partial scattering density is proportional to the total density:

$$
R_{s i}\left(E^{\prime}\right)=\frac{\Sigma_{s i}\left(E^{\prime}\right)}{\Sigma_{s}\left(E^{\prime}\right)} R_{s}\left(E^{\prime}\right) \quad \text { with } \quad \Sigma_{s}\left(E^{\prime}\right)=\sum_{i} \Sigma_{s i}\left(E^{\prime}\right)
$$

the asymptotic solution to this equation is expressed as:

$$
R_{S}(E)=\frac{S}{\left(\sum_{i} \Sigma_{s i}(E) \xi_{i}\right) \frac{E}{\Sigma_{s}(E)}} .
$$

Thus, the slowing-down power of a mixture of isotopes is given by:

$$
\bar{\xi}(E)=\frac{\sum_{i} \Sigma_{s i}(E) \xi_{i}}{\Sigma_{s}(E)}
$$

The asymptotic flux is thus obtained by the usual $1 / E$ formula (assuming that the variation in $\xi$ is insignificant):

$$
\Phi(E)=\frac{S}{\xi \Sigma_{s}(E) E} \quad \text { or else } \quad \Phi(u)=\frac{S}{\xi \Sigma_{s}(u)}
$$

For an absorbing medium, the scattering cross section can be substituted by the total cross section. When far enough from the resonances, the scattering cross section may be replaced by the potential cross section, $\Sigma_{p}$, which is of practically constant versus energy. If the medium is a mixture of heavy nuclei (uranium) and light nuclei (hydrogen and oxygen from water), the flux spectrum is governed by the heavy nuclei in the fast energy region, close to the energy at which neutrons are emitted since collisions with these heavy nuclei induce a slight increase in lethargy. Light nuclei, however, chiefly influence the epithermal and thermal parts since most scattering collisions with hydrogen result in high energy loss. The stationary neutron flux verifies the Boltzmann integro-differential equation for a mixture, assuming isotropic scattering:

$$
\begin{aligned}
& \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, u)+\Sigma_{t}(\vec{r}, u) \Phi(\vec{r}, \vec{\Omega}, u) \\
& =\sum_{k \text { constituents }} \int_{u-\varepsilon_{k}}^{u} d u^{\prime} \int_{4 \pi} d \Omega^{\prime} \Sigma_{s}^{k}\left(\vec{r}, u^{\prime}\right) \times P\left(\vec{\Omega} \cdot \overrightarrow{\Omega^{\prime}}, u \rightarrow u^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}, u^{\prime}\right)+S(\vec{r}, \vec{\Omega}, u)
\end{aligned}
$$

### 4.4 Slowing Down in an Absorbing Medium

(Ferziger and Zweifel 1966, p82)
Let us first consider the case of weak absorption localized in terms of space and energy, as occurs for instance with a sufficiently thin sheet of absorbing material (e.g. cadmium, indium or aluminium). Such set-ups exist in detectors like Mobile Fission Chambers (MFC), which have a coating of fissile uranium, which are introduced through the bottom of the vessel into the instrumentation thimble of $P W R$ assemblies to measure activity. It is assumed that the flux spectrum $\Phi(E)$ is not disturbed by the presence of the detector in the fission chamber (although this necessarily affects the geometrical design of the detector given the perpetual dilemma of instrumentation design: to measure without disturbing the phenomenon by the act of measurement itself!). Hence, the detector absorption rate is:
$R_{a}=\int_{0}^{E_{0}} \Sigma_{a}(E) \Phi(E) d E=N_{a} \int_{0}^{E_{0}} \sigma_{a}(E) \Phi(E) d E \quad$ absorptions per $\mathrm{cm}^{3}$ and per second
In the continuous slowing-down theory frame, the flux spectrum may be substituted by $S /\left(\bar{\xi} \Sigma_{s}(E)\right)$. Supposing that the slowing-down cross section is
constant as a first-order approximation, which is approximately verified for industrial moderators, the following is obtained:

$$
R_{a}=\frac{N_{a} S}{\bar{\xi} \Sigma_{s}} \int_{0}^{E_{0}} \sigma_{a}(E) \frac{d E}{E}=\frac{N_{a} S}{\bar{\xi} \Sigma_{s}} I_{a}^{\infty}
$$

This formulation introduces the concept of the infinite dilution resonance integral:

$$
I_{a}^{\infty}[b a r n] \equiv \int_{0}^{E_{0}} \sigma_{a}(E) \frac{d E}{E}
$$

for a given nuclide (the absorbing nucleus of the detector in the considered example). These values are given in nuclear data banks such as JEF2 (Table 4.3):

The resonance integral allows comparison of the intrinsic absorption power of a single nuclide placed in a diffusing medium. It should be noted that $R_{a}$ leads to the value $S$, i.e. the slowing-down density in a purely scattering medium since $q(u)=S$. Let us suppose now that absorption is homogeneous in space and energy (as for industrial moderators), and there is a point source at lethargy $u_{0}$. The neutron balance must account for neutron loss at lethargy $u$ :

$$
\int_{u^{\prime}=u_{0}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\Sigma_{t}(u) \Phi(u) \equiv \Sigma_{s}(u) \Phi(u)+\Sigma_{a}(u) \Phi(u)
$$

The total reaction rate can be introduced in the integral term by expressing $\Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right)$ in the obvious form $\Sigma_{t}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) \Sigma_{s}\left(u^{\prime}\right) / \Sigma_{t}\left(u^{\prime}\right)$, where $\Sigma_{s}\left(u^{\prime}\right) / \Sigma_{t}\left(u^{\prime}\right)$ represents the scattering probability. The quantity $S \Sigma_{s}\left(u_{0}\right) / \Sigma_{t}\left(u_{0}\right)$ signifies the fact that only neutrons emitted by the source and not absorbed may scatter. $P\left(u_{0} \rightarrow u\right)$ $=e^{-\left(u-u_{0}\right)} /(1-\alpha)$ is the probability for a neutron emitted at lethargy $u_{0}$ of reaching lethargy $u$. Hence:

$$
\int_{u^{\prime}=u_{0}}^{u} R_{t}\left(u^{\prime}\right) \frac{\Sigma_{s}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\int_{u^{\prime}=u-\varepsilon}^{u} R_{t}\left(u^{\prime}\right) \frac{\Sigma_{s}\left(u^{\prime}\right)}{\Sigma_{t}\left(u^{\prime}\right)} P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=R_{t}(u)
$$

In the case of hydrogen $(\alpha=1, \varepsilon=+\infty)$, this equation is written in energy terms as:

Table 4.3 Infinite dilution resonance integral for some notable nuclides

|  | ${ }_{92}^{235} U$ | ${ }_{49}^{115} \mathrm{In}$ | ${ }_{48}^{113} \mathrm{Cd}$ | ${ }_{54}^{135} \mathrm{Xe}$ |
| :--- | :--- | :--- | :--- | :--- |
| $I_{a}^{\infty}[$ barn $]$ (JEF2.2) | 403.67 | 3223.11 | 394.07 | 7663.79 |

$$
\int_{-\infty}^{E} R_{t}\left(E^{\prime}\right) \frac{\Sigma_{s}\left(E^{\prime}\right)}{\Sigma_{t}\left(E^{\prime}\right)} \frac{1}{E^{\prime}} d E^{\prime}=R_{t}(E)
$$

Differentiating this equation wrt.E:

$$
R_{t}(E) \frac{\Sigma_{s}(E)}{E \Sigma_{t}(E)}=\frac{d R_{t}(E)}{d E}
$$

which by integration gives: $R_{t}(E)=C e^{\int_{E}^{E_{0}} \frac{S_{s}\left(E^{\prime}\right)}{\Sigma_{t}\left(E^{\prime}\right)} \frac{d E^{\prime}}{E^{\prime}}}=C e^{\int_{E}^{E_{0}} \frac{\Sigma_{t}\left(E^{\prime}\right)-\Sigma_{a}\left(E^{\prime}\right)}{\Sigma_{t}\left(E^{\prime}\right)} \frac{d d E^{\prime}}{E^{\prime}}}=C \frac{E_{0}}{E} e^{-\int_{E}^{-\frac{\Sigma_{a}\left(E^{\prime}\right)}{E_{t}\left(E^{\prime}\right)} \frac{d d{ }^{\prime}}{E^{\prime}}}}$
The constant $C$ can be deduced by carrying out the neutron balance at the origin of lethargies, where the reaction rate tends towards the first collision scattering rate:

$$
\underbrace{S \frac{\Sigma_{s}\left(E_{0}\right)}{\Sigma_{t}\left(E_{0}\right)} \frac{1}{E_{0}}}_{\begin{array}{l}
\text { neutrons } \\
\text { scattering } \\
\text { at } E_{0}
\end{array}}+\lim _{u \rightarrow u_{0}} \underbrace{u}_{0} R_{t}\left(u^{\prime}\right) \frac{\Sigma_{s}\left(u^{\prime}\right)}{\nu_{t}\left(u^{\prime}\right)} P\left(u^{\prime} \rightarrow u_{0}\right) d u^{\prime}=R_{t}\left(u_{0}\right)=C \frac{E_{0}}{E_{0}}
$$


Compared to cases without absorption, this solution contains the multiplying term:

$$
p(E) \equiv \frac{\Sigma_{s}\left(E_{0}\right)}{\Sigma_{t}\left(E_{0}\right)} e^{-\int_{E}^{E_{0}} \frac{\Sigma_{a}\left(E^{\prime}\right)_{d E^{\prime}}}{\Sigma_{t}\left(E^{\prime}\right) E^{\prime}}}
$$

which is the probability for a neutron born at energy $E_{0}$ of escaping absorption and reaching energy $E$. Physical reasoning may be used to obtain an order of magnitude of $p(u)$ : variations in slowing-down density are caused strictly by neutron loss in accordance with the absorption rate. Furthermore, the slowingdown density may be approximated in a homogeneous medium by:

$$
\begin{aligned}
& \left\{\begin{array}{l}
q(u) \approx \xi\left(\Sigma_{s}+\Sigma_{a}(u)\right) \Phi(u) \\
d q(u)=-\Sigma_{a}(u) \Phi(u)
\end{array} \Rightarrow \frac{d q}{q(u)} \approx-\frac{\Sigma_{a}(u)}{\xi\left(\Sigma_{s}+\Sigma_{a}(u)\right)} \Rightarrow p(u)\right. \\
& \quad=\frac{q(u)}{q(0)} \approx e^{-\int_{0}^{u} \frac{\Sigma_{a}(u)}{\xi\left(\Sigma_{s}+\Sigma_{a}(u)\right)} d u}
\end{aligned}
$$

The resonance escape probability factor $p$ is defined as the probability for a neutron of reaching thermal energy $E_{t h}$ without being absorbed in the medium, principally by the resonances of heavy-nuclei cross sections:

$$
p \equiv p_{\left(E_{t h}=0,0253 \quad e V\right)} \equiv \frac{\Sigma_{s}\left(E_{0}\right)}{\Sigma_{t}\left(E_{0}\right)} e^{-\int_{E_{t h}}^{E_{0}} \frac{\Sigma_{a}\left(E^{\prime}\right) d E^{\prime}}{\Sigma_{t}\left(E^{\prime}\right) E^{\prime}}}
$$

The factor $1-p$ is thus a measure of the amount of neutrons absorbed chiefly by the resonances. Slowing-down by hydrogen with an absorption term characterizes quite satisfactorily a hydrogenated medium with an infinite mass. Actually, hydrogen is weakly absorbing, whereas scattering collision with heavy nuclei causes slight loss of neutron energy. For slowing-down by a nuclide heavier than hydrogen, there is no analytical solution, and the problem must be solved numerically with the help of computers. For the particular case where $\Sigma_{a}(E) / \Sigma_{s}(E) \approx C$ is almost constant, a further analytical solution can be applied. Introducing this condition into the slowing-down differential equation gives:

$$
\left\{\begin{array}{l}
\frac{d q(u)}{d u}=-\Sigma_{a}(u) \Phi(u)=S(u)-C \Sigma_{s}(u) \Phi(u)=-C R_{s}(u) \\
\text { with } \quad q(u)=\int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=u} R_{S}\left(u^{\prime}\right) d u^{\prime} \int_{u^{\prime \prime}=u}^{u^{\prime \prime}=u^{\prime}+\varepsilon} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}
\end{array}\right.
$$

for which the asymptotic solution far from the source may be written as $q(u)=$ $q_{0} e^{-m u}=S e^{-m u}$

By substituting $R_{S}\left(u^{\prime}\right)$ by $-\frac{1}{C} \frac{d q\left(u^{\prime}\right)}{d u^{\prime}}$, a transcendental equation in $m$ is obtained:

$$
\begin{aligned}
q_{0} e^{-m u} & =\int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=u} \frac{1}{C} q_{0} m e^{-m u^{\prime}} d u^{\prime} \int_{u^{\prime \prime}=u}^{u^{\prime \prime}=u^{\prime}+\varepsilon} \frac{e^{-\left(u^{\prime \prime}-u^{\prime}\right)}}{1-\alpha} d u^{\prime \prime} \\
& =q_{0} \frac{m}{C(1-\alpha)} \int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=u} e^{-m u^{\prime}}\left(e^{-\left(u-u^{\prime}\right)}-\alpha\right) d u^{\prime}
\end{aligned}
$$

$$
\begin{aligned}
e^{-m u} & =\frac{m}{C(1-\alpha)} \int_{u^{\prime}=u-\varepsilon}^{u^{\prime}=u}\left(e^{-m u^{\prime}} e^{-\left(u-u^{\prime}\right)}-\alpha e^{-m u^{\prime}}\right) d u^{\prime} \\
& =\frac{m}{C(1-\alpha)}\left[\frac{e^{-m u}}{m-1}\left(\frac{1}{\alpha^{m-1}}-1\right)-\frac{\alpha e^{-m u}}{m}\left(\frac{1}{\alpha^{m}}-1\right)\right] \\
1 & =\frac{m}{C(1-\alpha)}\left[\frac{1}{m-1}\left(\frac{1}{\alpha^{m-1}}-1\right)-\frac{\alpha}{m}\left(\frac{1}{\alpha^{m}}-1\right)\right]
\end{aligned}
$$

thus, the transcendental equation over $m$ :

$$
\frac{m}{(1-\alpha)}\left[\frac{1}{m-1}\left(\frac{1}{\alpha^{m-1}}-1\right)-\frac{\alpha}{m}\left(\frac{1}{\alpha^{m}}-1\right)\right]=\frac{1}{(1-\alpha)(m-1)}\left[\frac{1}{\alpha^{m-1}}-m+\alpha(m-1)\right]=C
$$

Using the moments of the slowing-down probability density $P(0 \rightarrow u)$ :

$$
\int_{u=0}^{u=\varepsilon} P(0 \rightarrow u) d u=1, \overline{\Delta u} \equiv \int_{u=0}^{u=\varepsilon} u P(0 \rightarrow u) d u=\xi, \overline{\Delta u^{2}} \equiv \int_{u=0}^{u=\varepsilon} u^{2} P(0 \rightarrow u) d u=2 \xi \gamma
$$

with $C=\int_{u=0}^{u=\varepsilon} P(0 \rightarrow u) \quad e^{m u} d u-1$ and expansion into a Taylor series up to order 2 of $e^{m u} \approx 1+m u+\frac{m^{2} u^{2}}{2}$, the following equation is obtained:

$$
C=m \xi+m^{2} \xi \gamma \quad \text { i.e. } \quad m \approx \frac{C}{\xi}-\frac{\gamma C^{2}}{\xi^{2}}=\frac{\Sigma_{a}}{\xi \Sigma_{s}}\left(1-\frac{\gamma \Sigma_{a}}{\Sigma_{s}}\right) \approx \frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}}
$$

This approximate result is found by computing the total reaction rate, given by:

$$
\begin{aligned}
R_{t}(u) & =\int_{u-\varepsilon}^{u} R_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime}=\int_{u-\varepsilon}^{u} \frac{\Sigma_{s}(u)}{\Sigma_{t}(u)} R_{t}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime} \\
& =\int_{u-\varepsilon}^{u} \frac{1}{1+C} R_{t}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime}
\end{aligned}
$$

the solution of which is of the form $R_{t}(u)=A e^{-m u}$. Since:

$$
\frac{d q(u)}{d u}=-m q_{0} e^{-m u}=-C R_{s}(u)=-C \frac{\Sigma_{s}}{\Sigma_{t}} R_{t}(u)=-\frac{C}{1+C} A e^{-m u}
$$

it can be deduced that: $A=m q_{0} \frac{1+C}{C}$
If absorption is weak, the energy attenuation of the slowing-down density is also weak. Thus, $m$ is small compared to 1 , thereby justifying the expansion of $q(u)=$ $q_{0} e^{-m u}$ into a Taylor series around 0 . Finally, the following equation is obtained:

$$
m=\frac{1}{\xi} \frac{C}{1+C}+\frac{\xi-\gamma}{\xi^{2}}\left(\frac{C}{1+C}\right)^{2}+\ldots=\frac{1}{\xi} \frac{\Sigma_{a}}{\Sigma_{t}}+\frac{\xi-\gamma}{\xi^{2}}\left(\frac{\Sigma_{a}}{\Sigma_{t}}\right)^{2}+\ldots
$$

where $\gamma \equiv \overline{\Delta u^{2}} / 2 \xi$ characterizes the order 2 moment of the scattering law (Reuss 2008, p219). At first order, the following relations are found:

$$
q(u)=q_{0} e^{-m u}=S e^{-\frac{1}{\xi} \frac{\Sigma a}{\Sigma_{t}} u} \quad \text { and } \quad R_{s}(u)=q(u) / \xi
$$

for slowing-down in a non-absorbing medium. At order 2, and assuming that $(\xi-\gamma) \sum_{a}$ is insignificant compared to $\xi \sum_{s}(\gamma$ is very close to $\xi)$, the equations are:

$$
q(u)=S e^{-\frac{\Sigma_{a}}{\xi \sum_{s}+\gamma \Sigma_{a}} u} \quad \text { and } \quad R_{t}(u)=\frac{\Sigma_{s}+\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} q(u)
$$

The Wigner approximation then consists in assuming that $q(u)=S e^{-\int_{0}^{u} \frac{\sum_{a}}{\delta \Sigma_{t}} d u^{\prime}}$.

### 4.4.1 Slowly Varying Absorption: The Greuling-Goertzel Model

(Ferziger and Zweifel 1966, pp. 91 and 161)
The slowing-down density is given by:

$$
q(u)=\int_{0}^{u} R\left(u^{\prime}\right) d u^{\prime} \int_{-\infty}^{u} P\left(u^{\prime} \rightarrow u^{\prime \prime} \leq u+\varepsilon\right) d u^{\prime \prime}=\int_{u-\varepsilon}^{u} R\left(u^{\prime}\right) \frac{\left(e^{-\left(u-u^{\prime}\right)}-\alpha\right)}{1-\alpha} d u^{\prime}
$$

Assuming that the reaction rate $R\left(u^{\prime}\right)$ varies slowly owing to a slowly-varying absorption process, a first order expansion may be written as:

$$
R\left(u^{\prime}\right) \approx R(u)+\left(u^{\prime}-u\right) \frac{d R}{d u}
$$

Thus, the slowing-down density can be computed as:

$$
\begin{aligned}
q(u) & \approx \int_{u-\varepsilon}^{u} \frac{1}{1-\alpha}\left[R(u)+\left(u^{\prime}-u\right) \frac{d R}{d u}\right]\left[e^{-\left(u-u^{\prime}\right)}-\alpha\right] d u^{\prime} \\
& =\underbrace{\left(1-\frac{\alpha \varepsilon}{1-\alpha}\right)}_{\xi} R(u)-\underbrace{\left(1-\frac{\alpha}{1-\alpha} \varepsilon-\frac{\alpha}{1-\alpha} \frac{\varepsilon^{2}}{2}\right)}_{\gamma \xi} \frac{d R}{d u}
\end{aligned}
$$

Or even: $q(u)=\xi R(u)-\xi \gamma \frac{d R(u)}{d u}$ with $\xi=1-\frac{\alpha}{1-\alpha} \varepsilon$ and $\gamma=1-\frac{\alpha}{1-\alpha} \frac{\varepsilon^{2}}{2}$

Differentiating the integral expression of $q(u)$ leads to:

$$
\frac{d q(u)}{d u}=\frac{d}{d u}\left(\int_{u-\varepsilon}^{u} R\left(u^{\prime}\right) \frac{\left(e^{-\left(u-u^{\prime}\right)}-\alpha\right)}{1-\alpha} d u^{\prime}\right)=R(u)-\frac{1}{1-\alpha} \int_{u-\varepsilon}^{u} R\left(u^{\prime}\right) e^{-\left(u-u^{\prime}\right)} d u^{\prime}
$$

Using the Taylor series expansion of $R\left(u^{\prime}\right)$ in the integral term, the differential equation obtained is:

$$
\frac{d q(u)}{d u}=\xi \frac{d R(u)}{d u}
$$

Since $R(u)=\Sigma_{s}(u) \Phi(u)$ and without any source at lethargy $u$, $d q(u) /$ $d u=-\Sigma_{a}(u) \Phi(u)$, by substitution:

$$
q(u)=\xi R(u)-\xi \gamma \frac{d R(u)}{d u}=\xi R(u)-\gamma \frac{d q(u)}{d u}=\xi \Sigma_{s}(u) \Phi(u)+\gamma \Sigma_{a}(u) \Phi(u)
$$

Giving the flux expression in the model of Eugene Greuling ${ }^{20}$ and Gerald Goertzel ${ }^{21}$ :

$$
\begin{equation*}
\text { Greuling-Goertzel model : } \quad \Phi(u)=\frac{q(u)}{\xi \Sigma_{s}(u)+\gamma \Sigma_{a}(u)} \tag{4.21}
\end{equation*}
$$

It may be seen that, in the case of $\gamma=\xi$, the Wigner approximation $\Phi(u)=q(u) /$ $\left(\xi \Sigma_{t}(u)\right)$ is found, and if absorptions are considered to be weak compared to scattering, the Fermi model $\Phi(u)=q(u) /\left(\xi \Sigma_{s}(u)\right)$ is obtained. The GreulingGoertzel model for a source at zero lethargy leads to:

[^77]$$
q(u)=S e^{-\int_{0}^{u} \frac{\Sigma_{a}}{\overline{\xi \Sigma_{s}+\gamma \Sigma_{a}} d u^{\prime}}}
$$

The zeroth moment of the Boltzmann equation with $P_{1}$ approximation contains the slowing-down rate due to elastic scattering ( $R_{0}[]$, brackets stand for operator):

$$
R_{0}\left[\Phi_{0}(u)\right] \equiv \int_{u^{\prime}} \Sigma_{s, 0}\left(u^{\prime} \rightarrow u\right) \Phi_{0}\left(u^{\prime}\right) d u^{\prime}=\sum_{\text {constituents } i} \int_{u^{\prime}-\varepsilon_{i}}^{u} \Sigma_{s, 0}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha_{i}} \Phi_{0}\left(u^{\prime}\right) d u^{\prime}
$$

A constituent $i$ contributes to the slowing-down density as follows:

$$
q^{i}(u) \equiv \int_{u^{\prime}-\varepsilon_{i}}^{u} \Sigma_{s, 0}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}-\alpha_{i}}{1-\alpha_{i}} \Phi_{0}\left(u^{\prime}\right) d u^{\prime}
$$

By differentiation of this quantity, the following equation is found:
$\frac{d q^{i}(u)}{d u}=\Sigma_{s, 0}\left(u^{\prime}\right) \Phi_{0}\left(u^{\prime}\right)-\int_{u^{\prime}-\varepsilon_{i}}^{u} \Sigma_{s, 0}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha_{i}} \Phi_{0}\left(u^{\prime}\right) d u^{\prime}=\Sigma_{s, 0}\left(u^{\prime}\right) \Phi_{0}\left(u^{\prime}\right)-R_{0} \Phi_{0}(u)$
Similarly, the first moment of the Boltzmann equation introduces the anisotropic slowing-down density by elastic scattering ( $R_{1}[]$ operator and current $\Phi_{1}$, scattering angle $\mu$ in the laboratory frame):

$$
R_{1}\left[\Phi_{1}\right](u, \mu) \equiv \int_{u^{\prime}} \Sigma_{s, 1}\left(u^{\prime} \rightarrow u\right) \Phi_{1}\left(u^{\prime}\right) d u^{\prime}=\sum_{\text {constituents }} \int_{u^{\prime}-\varepsilon_{i}}^{u} \mu \Sigma_{s, 0}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha_{i}} \Phi_{1}\left(u^{\prime}\right) d u^{\prime}
$$

The anisotropic slowing-down density is defined as:

$$
q_{1}^{i}(u, \mu) \equiv \int_{u^{\prime}-\varepsilon_{i}}^{u} \mu \Sigma_{s, 0}\left(u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}-\alpha_{i}}{1-\alpha_{i}} \Phi_{1}\left(u^{\prime}\right) d u^{\prime}
$$

For non-absorbing hydrogen $(\alpha=0)$, the slowing-down rate is strictly equal to the slowing-down density, which leads to a completely analytical solution (Silvennoinen 1976, p145):

$$
\left\{\begin{array}{l}
\frac{d q^{H}(u)}{d u}=\Sigma_{s}^{H}\left(u^{\prime}\right) \Phi_{0}\left(u^{\prime}\right)-q^{H}(u) \\
\frac{d q_{1}^{H}(u)}{d u}=\Sigma_{s}^{H}\left(u^{\prime}\right) \Phi_{1}\left(u^{\prime}\right)-\frac{3}{2} q_{1}^{H}(u)
\end{array}\right.
$$

For other isotopes, the Greuling-Goertzel formalism is applied. As seen earlier, this model implies that:

$$
q_{i}(u)+\gamma_{i} \frac{d q_{i}(u)}{d u}=\xi_{i} R^{i}(u)=\xi_{i} \Sigma_{s}^{i} \Phi_{0}(u)
$$

The solution to this equation is a first-order approximation of the slowing-down density:

$$
\xi_{i}=1-\frac{\alpha_{i}}{1-\alpha_{i}} \ln \frac{1}{\alpha_{i}} \quad \text { and } \quad \gamma_{i}=\frac{1}{2 \xi_{i}} \int_{u-\varepsilon_{i}}^{u}\left(u-u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha_{i}} d u^{\prime}
$$

For anisotropic slowing-down, the following equation is written:

$$
q_{1}^{i}(u, \mu)+\lambda_{i} \frac{d q_{1}^{i}(u, \mu)}{d u}=\omega_{i} \Sigma_{s}^{i} \Phi_{1}(u)
$$

with: $\omega_{i}=\int_{u-\varepsilon_{i}}^{u} \mu\left(u-u^{\prime}\right) \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha_{i}} d u^{\prime}$ and $\lambda_{i}=\frac{1}{2 \omega_{i}} \int_{u-\varepsilon_{i}}^{u} \mu\left(u-u^{\prime}\right)^{2} \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha_{i}} d u^{\prime}$
Each nuclide can be considered separately or all the nuclides can be computed at the same time in a homogeneous approximation (except hydrogen which can be computed exactly) using the mean values of $\gamma$ and $\lambda$ :

$$
\overline{\gamma(u)}=\frac{\sum_{i} \gamma_{i}(u) \xi_{i}(u) \Sigma_{s}^{i}(u)}{\sum_{i} \xi_{i}(u) \Sigma_{s}^{i}(u)} \quad \text { and } \quad \overline{\lambda(u)}=\frac{\sum_{i} \lambda_{i}(u) \omega_{i}(u) \Sigma_{s}^{i}(u)}{\sum_{i} \omega_{i}(u) \Sigma_{s}^{i}(u)}
$$

### 4.4.2 Slowing Down in a Medium with a Resonant Cross Section

For low energies, a resonance may be thought as a "trap" of lethargy width $\Delta u$ that absorbs any neutron found inside it (considered as a black trap), or even as a negative monoenergetic source $S(u)=-S \delta\left(u-u_{R}\right) . \quad u_{R}$ is the lethargy
corresponding to the resonance, thereby leading to a flux discontinuity at $u=u_{R}+\varepsilon$. An analogy can be drawn with age distribution by age group, where a very marked decrease was seen in the infant age group during the both World Wars as men died in action and the birth rate decreased (in this case, $\varepsilon$ is equivalent to the age of reproduction, i.e. around 25 years here). In theory, a depletion occurs once more at 50 years $(\approx 2 \varepsilon)$ but it is in fact far less pronounced due to smoothing over time. Supposing that resonance is modeled as a trap of infinite depth and of width $\Gamma$ in lethargy units, the slowing-down density crossing the resonance located at $u_{R}$ is given by:

$$
q\left(u_{R}\right)=\int_{-\infty}^{u_{R}} R_{S}\left(u^{\prime}\right) d u^{\prime} \int_{u_{R}}^{+\infty} P\left(u^{\prime} \rightarrow u^{\prime \prime}\right) d u^{\prime \prime}
$$

Taking the origin of lethargies to be at the entrance/beginning of the trap and in the case of the asymptotic state $\left(R_{s}(u)=S / \xi\right)$, the number of neutrons falling into the trap, and hence, by definition, the complementary to 1 of the resonance escape probability after renormalization to the source, we have:

$$
1-p=\int_{0}^{\Gamma} \frac{1}{\xi} d u^{\prime} \int_{u^{\prime}-\varepsilon}^{0} \frac{e^{-\left(u^{\prime}-u^{\prime \prime}\right)}}{1-\alpha} d u^{\prime \prime}=\int_{0}^{\Gamma} \frac{1}{\xi} d u^{\prime} \frac{e^{-u^{\prime}}-\alpha}{1-\alpha}=\frac{1-e^{-\Gamma}-\alpha \Gamma}{\xi(1-\alpha)}
$$

If $\Gamma>\varepsilon$, absolutely no neutrons can escape from the trap, thus $p=0$ (Fig. 4.17).
If $\Gamma$ is small enough, $e^{-\Gamma}$ can be expanded in a Taylor series leading to $1-p \approx \Gamma / \xi$, and the number of neutrons absorbed by the trap is thus identical to the number reaching the lethargy band $\Gamma$ under the asymptotic hypothesis $R_{s}=\Gamma / \xi$.

Fig. 4.17 Trap of width $\Gamma$


The impact on the spectrum beyond lethargy $u_{R}$ is very small. If the trap is not "black" but "grey", i.e. some neutrons have a non-zero probability of escaping absorption, the resonance escape probability is given with satisfactory prediction by:

$$
p(E) \approx e^{-\int_{E}^{E_{0}} \frac{\Sigma_{a}\left(E^{\prime}\right)}{\xi \Sigma_{t}\left(E^{\prime}\right)} \frac{d E^{\prime}}{E^{\prime}}}
$$

For a set of resonances, the escape probabilities are multiplicative assuming that they do not interfere with each other. Furthermore, assuming that $\Sigma_{s}$ is independent of energy, the integrated escape probability simplifies to:

$$
p\left(E_{t h}\right)=e^{-\frac{N_{a}}{\overline{\delta s} s} \int_{E_{t h}}^{E_{0}} \frac{\sigma_{a}\left(E^{\prime}\right)}{1+\frac{N_{a} a\left(E^{\prime}\right)}{\Sigma_{s}}} \frac{d E^{\prime}}{E^{\prime}}}
$$

the integral form of which tends to the infinite dilution resonance integral $\int_{0}^{\infty} \sigma_{a}$ (E) $d E / E$ where the dilution factor $N_{s} / N_{a}$ tends to infinity. The slowing-down density can be computed from the differential equation seen previously:

$$
\frac{d q(u)}{d u}=-\Sigma_{a}(u) \Phi(u)=-\Sigma_{a}(u) \frac{q(u)}{\xi \Sigma_{s}(u)+\gamma \Sigma_{a}(u)}
$$

Its solution is:

$$
\ln \frac{1}{q(u)}=\int_{0}^{u} \frac{\Sigma_{a}\left(u^{\prime}\right)}{\xi \Sigma_{s}\left(u^{\prime}\right)+\gamma \Sigma_{a}\left(u^{\prime}\right)} d u^{\prime}
$$

Outside the resonance, the absorption and scattering cross sections are almost constant. Therefore, the slowing-down density out of the trap is computed as:

$$
\left\{\begin{array}{l}
\ln \frac{1}{q(u)}=\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u \quad \text { for } \quad u<u_{R} \\
\ln \frac{1}{q(u)}=\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u+\frac{\Gamma}{\xi} \quad \text { for } \quad u>u_{R}+\Gamma
\end{array}\right.
$$

where $\Gamma / \xi$ is the number of neutrons lost inside the trap. Hence, by assuming that absorption occurs only in the resonance:

$$
\left\{\begin{array}{c}
q(u)=e^{-\frac{\Sigma_{a}(u)}{\xi \Sigma_{s}(u)} u} \quad \text { for }
\end{array} \quad 0<u<u_{R}, ~(u)=e^{-\frac{\Sigma_{a}(u)}{\xi \Sigma_{s}(u)} u} e^{-\frac{\Gamma}{\xi}} \quad \text { for } \quad u_{R}+\Gamma<u\right.
$$

Inside the resonance, the cross section is assumed to be infinite, thus:

$$
\int_{u_{R}}^{u_{R}+\Gamma} \frac{\Sigma_{a}\left(u^{\prime}\right)}{\xi \Sigma_{s}\left(u^{\prime}\right)+\gamma \Sigma_{a}\left(u^{\prime}\right)} d u^{\prime} \approx \int_{u_{R}}^{u_{R}+\Gamma} \frac{1}{\gamma} d u^{\prime}=\frac{\Gamma}{\gamma}
$$

### 4.4.3 Inelastic Slowing-Down

While the literature on elastic slowing-down theory is copious, theoretical works on inelastic slowing down are less common. In 1968, the approach of Martine Pujol, ${ }^{22}$ developed when she was working at the famous "Service de Mathématiques

[^78]
(Courtesy La Recherche)

Appliquées" (CEA) headed by Jean Bussac, ${ }^{23}$ resulted in a simple and elegant method for solving several problems in a semi-analytical manner. Her method allowed the introduction of an analytical consideration inside a wide energy group. While the increasing use of computational power superseded the use of analytical models for fine multigroup calculations, Pujol's analytical model provides a more didactic understanding of inelastic slowing-down.

By the end of the 60's, the multigroup approach became more widespread but physical models with energy as a variable nevertheless remained in use. Martine Pujol worked on slowing-down in plutonium oxides by combining the inelastic problem for plutonium with the elastic problem for oxygen. ${ }^{24}$

The slowing-down operator (in brackets) is written as:

[^79]
(Courtesy Jean Bussac)
${ }^{24}$ Martine Pujol: Modèle approché pour la diffusion inélastique des neutrons rapides [Approximated model for inelastic scattering of fast neutrons], PhD thesis at the Faculty of Science, University of Orsay, 1968.
$$
R[\Phi(E)] \equiv \int_{E^{\prime}=E}^{E^{\prime}=+\infty} \Sigma_{s}\left(E^{\prime}\right) P\left(E^{\prime} \rightarrow E\right) \Phi\left(E^{\prime}\right) d E^{\prime}
$$

The inelastic transfer probability is approximated by:

$$
\tilde{P}\left(E^{\prime} \rightarrow E\right) \equiv \begin{cases}f\left(E^{\prime}\right) g(E) & \text { if } E^{\prime} \geq E \\ 0 & \text { if } E^{\prime}<E\end{cases}
$$

This approximated probability must satisfy certain normalization conditions:

$$
\int_{E=0}^{E=E^{\prime}} \tilde{P}\left(E^{\prime} \rightarrow E\right) d E=f\left(E^{\prime}\right) \int_{E=0}^{E=E^{\prime}} g(E) d E=1
$$

so as to conserve the integrated scattering cross section.

$$
\begin{aligned}
\tilde{R}\left[\Phi_{0}(E)\right] & \equiv \int_{E^{\prime}=E}^{E^{\prime}=+\infty} \tilde{P}\left(E^{\prime} \rightarrow E\right) \Sigma_{s}\left(E^{\prime}\right) \Phi_{0}\left(E^{\prime}\right) d E^{\prime} \\
& =\int_{E^{\prime}=E}^{E^{\prime}=+\infty} P\left(E^{\prime} \rightarrow E\right) \Sigma_{s}\left(E^{\prime}\right) \Phi_{0}\left(E^{\prime}\right) d E^{\prime}=R\left[\Phi_{0}(E)\right]
\end{aligned}
$$

This means that the approximated operator must be equal to the exact operator for a well-chosen reference flux. Conservation of the integrated scattering cross section leads to the conclusion that $\tilde{P}\left(E^{\prime} \rightarrow E\right)$ depends only on one function:

$$
\tilde{P}\left(E^{\prime} \rightarrow E\right) \equiv g(E) \int_{E^{\prime \prime}=0}^{E^{\prime \prime}=E^{\prime}} g\left(E^{\prime \prime}\right) d E^{\prime \prime}
$$

Using the function $h(E) \equiv \frac{1}{f(E)}$, which is positive and increases with energy, and which is equal to 0 for $E=0$ :

$$
\tilde{P}\left(E^{\prime} \rightarrow E\right)=\frac{\frac{d h}{d E}(E)}{h\left(E^{\prime}\right)}
$$

$h(E)$ is defined up to a constant which can be such that $h(+\infty)=1$. The function $h$ is computed from the exact operator by:

$$
Y(E) \equiv \frac{R[\Phi(E)]}{\frac{d h}{d E}(E)}=\int_{E^{\prime}=E}^{E^{\prime}=+\infty} \frac{\Sigma_{s}\left(E^{\prime}\right) \Phi\left(E^{\prime}\right)}{h\left(E^{\prime}\right)} d E^{\prime}
$$

Since:

$$
\frac{d(Y(E) h(E))}{d E}=R[\Phi(E)]-\Sigma_{s}(E) \Phi(E)
$$

the following equation is obtained:

$$
h(E)=h(+\infty) \exp \left(-\int_{E^{\prime}=E}^{E_{E^{\prime}=E^{\prime \prime}}^{E^{\prime}=+\infty}} \frac{R\left[\Phi\left(E^{\prime \prime}\right)\right]}{\Sigma_{s}^{\prime}=+\infty} \Sigma_{s}\left(E^{\prime}\right) \Phi\left(E^{\prime}\right)-R\left[\Phi\left(E^{\prime}\right)\right] \quad d E^{\prime \prime}\right)
$$

Pujol proposed the use of an approximated inelastic slowing-down operator introducing the concept of reduced inelastic lethargy $v$ or the generalized lethargy such that:

$$
\tilde{P}\left(v^{\prime} \rightarrow v\right)=e^{-\left(v-v^{\prime}\right)} \quad \text { for } \quad v^{\prime} \leq v
$$

where:

$$
\begin{equation*}
\text { Pujol inelastic lethargy : } \quad v(E)=-\ln (h(E)) \tag{4.22}
\end{equation*}
$$

The function $\tilde{P}\left(v^{\prime} \rightarrow v\right)$ behaves in exactly the same way as that for elastic slowing-down on hydrogen as a function of lethargy $u$. If slowing down is elastic and isotropic, then $v(E)=\frac{u(E)}{\xi}$ where $u(E)$ is the usual lethargy.

The mixed case of elastic and inelastic cross sections is modeled by:

$$
\widetilde{\Sigma}_{s}\left(E^{\prime} \rightarrow E\right)=\Sigma_{s, \text { inel }} \frac{\frac{d h_{\text {inel }}}{d E}(E)}{h_{\text {inel }}\left(E^{\prime}\right)}+\Sigma_{s, \text { elas }} \frac{\frac{d h_{\text {elas }}}{d E}(E)}{h_{\text {elas }}\left(E^{\prime}\right)}
$$

Pujol showed that the approximation:

$$
\widetilde{\Sigma}_{s}\left(E^{\prime} \rightarrow E\right)=\left(\Sigma_{s, \text { inel }}+\Sigma_{s, e l a s} \frac{\frac{d h}{d E}(E)}{h\left(E^{\prime}\right)}\right.
$$

is satisfactory in terms of precision. She computed $h(E)$ as a function of cross sections using an iterative flux calculation, starting with a given fission spectrum.

Assuming the inelastic slowing down to be characterized correctly by an analytical law, several space-dependent problems may be considered in a semi-
analytical manner, just as for thermalization. These works were published ${ }^{25}$ in 1967.

### 4.4.4 The $Q_{n}$ Slowing-Down Approximation

The standard analytical slowing-down models (Fermi in 1936, Wigner in 1955, Greuling-Goertzel in 1960, Pujol in 1967, etc.) were not sufficiently precise for fast neutrons in media with large inelastic scattering cross sections. Improvements were made in the 1970s, in particular through the use of numerical considerations in multigroup approximations.

In 1976, Brigitte Rocca-Volmerange ${ }^{26}$ proposed ${ }^{27}$ a generalization of the previous models to order $n$, using the global slowing-down parameters and a differential formalism of the integral form of the Boltzmann equation.

Let $\Psi(u, w)$ be the fraction of the slowing-down density $q(u)$, which arrives at lethargy $u^{\prime \prime}=u+w$, where $w$ is the minimum gain in lethargy attained by the neutrons:
$\Psi(u, w) \equiv \int_{u^{\prime}=-\infty}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime} \rightarrow u+w\right) \Phi\left(u^{\prime}\right) d u^{\prime}=\int_{u^{\prime}=-\infty}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u+w\right) \Phi\left(u^{\prime}\right) d u$
$\Psi(u, w)$ is called the minimum jump density. It is integrated from $u \equiv-\infty$ to avoid any problem of reference for lethargies. Differentiating the previous equation and supposing that $\Phi(-\infty)=0$, the following equation is obtained:

$$
\frac{\partial \Psi(u, w)}{\partial u}=\frac{\partial \Psi(u, w)}{\partial w}+\Sigma_{s}(u \rightarrow u+w) \Phi(u)
$$

Introducing the particular value of:

[^80]$$
\Psi(u, 0) \equiv R[\Phi(u)]=\int_{u^{\prime}=-\infty}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime}
$$

With the usual neutron balance equation:

$$
\Sigma_{t}(u) \Phi(u) \equiv R[\Phi(u)]+S(u)
$$

A differential form of the slowing-down equation $w r t . \Psi(u, w)$ is obtained:

$$
\frac{\partial \Psi(u, w)}{\partial u}=\frac{\partial \Psi(u, w)}{\partial w}+\frac{\Sigma_{s}(u \rightarrow u+w)}{\Sigma_{t}(u)}(\Psi(u, 0)-S(u))
$$

The moments of the function $\Psi(u, w)$ may now be defined, and are called the slowing-down density of order $n$ :

$$
q_{n}(u) \equiv \int_{w=0}^{w=\varepsilon} w^{m} \Psi(u, w) d w
$$

where $\varepsilon$ is the maximum gain in lethargy. By definition, $q_{0}(u) \equiv q(u)$, the usual slowing-down density. By successive differentiations wrt. lethargy, we get the following equations:

$$
\left\{\begin{array}{l}
\frac{d q_{0}(u)}{d u}=\Sigma_{s}(u) \Phi(u)-R[\Phi(u)] \\
\frac{d q_{n}(u)}{d u}=\int_{w=0}^{w=\varepsilon} w^{m} \Sigma_{s}(u) P(u \rightarrow u+w) d w-n q_{n-1}(u) \text { for } n>0
\end{array}\right.
$$

Using the transfer moments:

$$
\xi_{n}(u) \equiv \frac{\int_{w=0}^{w=\varepsilon} w^{m} \Sigma_{s}(u) P(u \rightarrow u+w) d w}{\Sigma_{s}(u)}=\int_{w=0}^{w=\varepsilon} w^{m} P(u \rightarrow u+w) d w
$$

and the scattering fraction:

$$
C_{s}(u) \equiv \frac{\Sigma_{s}(u)}{\Sigma_{t}(u)}
$$

the $\mathrm{Q}_{\mathrm{n}}$ system with $n+1$ differential equations is found:

$$
\left\{\begin{array}{l}
\frac{d q_{0}(u)}{d u}=C_{s}(u)(R[\Phi(u)]+S(u))-R[\Phi(u)] \\
\frac{d q_{j}(u)}{d u}=C_{s}(u) \xi_{j}(u)(R[\Phi(u)]+S(u))-j q_{j-1}(u) \quad \text { for } \quad 0<j \leq n
\end{array}\right.
$$

In reality, the fraction $\Psi(u, w)$ of the slowing-down density is significantly affected by the fact that the cross section $\Sigma_{s}\left(u^{\prime} \rightarrow u+w\right)$ either has discontinuities or sudden peak resonance values of inelastic cross sections. B. Rocca-Volmerange proposed that the function be made as regular as possible, enabling it to be approximated by a polynomial expansion:

$$
\frac{\Psi(u, w)}{\pi(u, w)} \approx \sum_{i=0}^{i=n} r_{i}(u) w^{i} \quad \text { and } \quad \frac{\widetilde{\Psi}(u, w)}{\pi(u, w)}=\sum_{i=0}^{i=n} r_{i}(u) w^{i}
$$

The weight function $\pi(u, w)$ used is the reference fraction $\bar{\Psi}(u, w)$ such that:

$$
\bar{\Psi}(u, w) \equiv \int_{u^{\prime}=-\infty}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime} \rightarrow u+w\right) \bar{\Phi}\left(u^{\prime}\right) d u^{\prime}
$$

$\bar{\Phi}(u)$ is here chosen as an arbitrary reference spectrum. These notations are generalized as:

$$
\widetilde{\Psi}(u, 0)=r_{0}(u) \bar{\Psi}(u, 0) \equiv r_{0}(u) R[\bar{\Phi}(u)]
$$

and $R[\widetilde{\Phi}(u)]=r_{0}(u) R[\bar{\Phi}(u)]$
Similarly:

$$
\tilde{q}_{j}(u)=\int_{w=0}^{w=+\infty} w^{j} \widetilde{\Psi}(u, w) d w=\sum_{i=0}^{i=n} r_{i}(u) \bar{q}_{i+j}(u)
$$

with:

$$
\bar{q}_{i+j}(u) \equiv \int_{w=0}^{w=+\infty} w^{i+j} \bar{\Psi}(u, w) d w=\int_{w=0}^{w=+\infty} w^{i+j} \int_{u^{\prime}=-\infty}^{u^{\prime}=u} \Sigma_{s}\left(u^{\prime} \rightarrow u+w\right) \bar{\Phi}\left(u^{\prime}\right) d u^{\prime}
$$

The functions $R[\widetilde{\Phi}(u)]$ and $\tilde{q}_{j}(u)$ are the unknowns of the $\mathrm{Q}_{\mathrm{n}}$ differential system previously established. By solving this system, all values of $\tilde{q}_{j}(u)$ may be computed using a linear inversion, allowing computation of the approximated spectrum $\widetilde{\Phi}(u)$ and $\widetilde{\Psi}(u, 0)$ :

$$
\widetilde{\Psi}(u, 0)=\sum_{i=0}^{i=n} Q_{i, n}(u) \tilde{q}_{i}(u) \quad \text { and } \quad \Psi(u, 0)=\sum_{i=0}^{i=n} Q_{i, n}(u) q_{i}(u)
$$

In the same way:

$$
R[\Phi(u)]=\sum_{i=0}^{i=n} Q_{i, n}(u) q_{i}(u)
$$

The Pujol and Cadilhac model described in the previous section represents the $\mathrm{Q}_{0}$ approximation. The $\mathrm{Q}_{1}$ approximation uses the first moment of the function $\Psi(u, w)$ :

$$
\Psi(u, 0)=Q_{0,1}(u) \int_{w=0}^{w=+\infty} \Psi(u, w) d w+Q_{1,1}(u) \int_{w=0}^{w=+\infty} w \Psi(u, w) d w
$$

The $n+1$ coefficients $Q_{i, n}(u)$, which are regular functions in lethargy, are solutions to:

$$
R[\bar{\Phi}(u)]=\bar{\Psi}(u, 0)=\sum_{i=0}^{i=n} Q_{i, n}(u) \bar{q}_{i}(u)
$$

This equation may be written in matrix form as:

$$
\left(\begin{array}{c}
\bar{\Psi}(u, 0) \\
0 \\
\vdots \\
0
\end{array}\right)=\left(\begin{array}{ccccc}
\bar{q}_{0}(u) & \cdot & \cdot & . & \bar{q}_{n}(u) \\
\cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot \\
\bar{q}_{n}(u) & \cdot & \cdot & . & \bar{q}_{2 n}(u)
\end{array}\right)\left(\begin{array}{c}
Q_{0, n}(u) \\
Q_{1, n}(u) \\
\vdots \\
Q_{n, n}(u)
\end{array}\right)
$$

The matrix is symmetrical and has $2 n+1 \bar{q}_{i}(u)$ terms.
The choice of the reference spectrum $\bar{\Phi}(u)$ was in fact independent of the true spectrum $\Phi(u)$ to be computed. Further, the functions $Q_{i, n}(u)$ are additive for a mixture of isotopes (weighted by the number of nuclides of the considered isotopes).

Computation of the $n+1 Q_{i, n}(u)$ functions is carried out using the $2 n+1 \bar{q}_{i}(u)$ reference functions, which are fitted on the $2 n+1$ physical parameters, namely the $2 n+1 \xi_{i}(u)$ moments. As $n$ increases, the importance of the reference spectrum used for weighting decreases, given that the number of moments increases as $2 n+1$. In practice, for $n=3$, the result does not depend on the reference spectrum used.

The approximated densities $\tilde{q}_{j}(u)$ satisfy the following differential system:

$$
\left\{\begin{array}{l}
\frac{d \tilde{q}_{0}(u)}{d u}=\left(C_{s}(u)-1\right)\left(\sum_{i=0}^{i=n} Q_{i, n}(u) \tilde{q}_{i}(u)\right)+C_{s}(u) S(u) \\
\frac{d \tilde{q}_{j}(u)}{d u}=C_{s}(u) \xi_{j}(u)\left(\sum_{i=0}^{i=n} Q_{i, n}(u) \tilde{q}_{i}(u)+S(u)\right)-j \tilde{q}_{j-1}(u) \quad \text { for } \quad 0<j \leq n
\end{array}\right.
$$

which can be integrated numerically using such approaches as the Euler or Runge-Kutta methods or Laplace transforms.

## Chapter 5 <br> Resonant Absorption

As discussed in previous chapters, the neutron interacts with the target nucleus as an incident wave. Indeed, the interaction probabilities at certain energies have a peaked shape due to quantum physics considerations. From the very inception of nuclear physics, more precise knowledge of cross sections as a function of energy and their modeling in a resonance zone were deemed essential. This is the goal of resonant absorption theory.
(Dresner 1960; Reactor Physics 1966) volume

### 5.1 Cross Section Model

### 5.1.1 Historical Background

Since the initial work by P. Kapur and Rudolph Peierls, ${ }^{1}$ several formalisms exist to describe cross sections as a function of incident particle energy, $\sigma(E)$, e.g. the Reich-Moore formalism or the Adler-Adler formalism. However, the most renowned formalism is that of Gregory Breit and Eugen Wigner (Photos 5.1 and 5.2). When resonances are separated (with no overlapping), the sum of contributions of single-level Breit-Wigner cross sections is sufficient. This model works for most nuclei, except for certain light nuclei or fissile nuclei in which the resonance width is not small compared to the energy spacing of the resonances. In this case, a multi-level formalism must be used.

[^81]Photo 5.1 A Hungarian stamp celebrating the physicist Eugen Wigner (The Marguet collection)


Photo 5.2 Gregory Breit (Public domain)


### 5.1.2 Intermediate Nucleus Theory

(Lilley 2001, p. 113)
The Breit-Wigner ${ }^{2}$ formalism is based on the process by which the intermediate nucleus, formed by interaction with the target nucleus, returns to ground state. In

[^82]the liquid-drop model discussed earlier in the section on fission, the collision of a neutron with a heavy nucleus such as ${ }^{238} U$ may lead to several possible configurations with various probabilities. The possible interactions are fission, radiative capture, elastic or inelastic scattering, or, more generally, any reaction. With inelastic scattering, the incident neutron energy is used to excite the compound nucleus, especially for heavy nuclei, which have a high density of excitation levels, in contrast with light nuclei, which have excessively high excitation levels. Where $\lambda$ is the decay constant (in $s^{-1}$ ) for a nucleus for a reaction from its excited state to its ground state (e.g. ${ }^{239} U^{*}$ in the case of neutron absorption by ${ }^{238} U$ ), the neutron lifetime is given by $\tau=1 / \lambda$. Each quantum state of the excited nucleus has a corresponding lifetime $\tau$, which represents the mean time during which the nucleus remains in this excited state. The decay probability, $\lambda$, is the sum of decay probabilities for partial decay in accordance with the other modes:
$$
\lambda=\lambda_{(n, f)}+\lambda_{(n, \gamma)}+\lambda_{\left(n, n^{\prime}\right)}
$$

A decaying nucleus is not in a precisely-known (deterministic) energy configuration. Using the Heisenberg ${ }^{3}$ uncertainty principle, $\Delta E \Delta t \geq \hbar, \Delta t$ represents the time period during which any measurement may be made. This time is limited by the mean nucleus lifetime, $\tau$.

The minimum precision for energy, i.e. mid-height width or total width, $\Delta E_{\min }=\Gamma_{[e V]}$, is thus related to the lifetime by the equation: $\Gamma \tau=\hbar=h /(2 \pi)$ (Fig. 5.1).

For each interaction type, it is thus possible to define the neutron width for resonant scattering, $\Gamma_{n}$, radiative capture, $\Gamma_{\gamma}$, and fission, $\Gamma_{f}$, as well as the widths for other possible reactions. Concepts of wave physics are used to describe the interaction: the impulse of the incident particle-target nucleus system is given by $p=\sqrt{2 \mu E}$, where $E$ is the total kinetic energy in the center-of-mass frame and $\mu$ is the reduced mass of the system $(1 / \mu=1 / M+1 / m)$. The reduced wavelength $\lambda$ is given by $\lambda=\hbar / p$. The partial widths, $\Gamma_{i}$, are related to the decay constants as follows:

[^83]Fig. 5.1 Effective cross section dependence with energy close to a resonance

$$
\Gamma_{i}=H \frac{1}{\tau_{i}}
$$

where $\lambda_{i}=\frac{1}{\tau_{i}}$ is the decay constant of the compound nucleus by reaction $i$.
The partial decay constants depend on the partial widths as follows:

$$
\frac{\lambda_{i}}{\lambda}=\frac{\Gamma_{i}}{\Gamma} \lambda=\lambda_{(n, \gamma)}+\lambda_{f}+\lambda_{\left(n, n^{\prime}\right)}+\ldots ; \quad \Gamma=\sum_{i} \Gamma_{i}
$$

In the compound nucleus model, the probabilities for the possible exit channels depend solely on the compound intermediate nucleus and not its mode of formation. Each channel is fully determined by dividing the compound nucleus into reactive pairs (e.g. ${ }_{92}^{235} U+{ }_{0}^{1} n$ or ${ }_{92}^{235} U+{ }_{0}^{1} n+\gamma$ which stem from the same excited nucleus), on the total angular momentum, $J$, the orbital angular momentum, $\ell$, and the spin angular momentum, $s$ (all expressed in terms of $\hbar$ ). The angular momenta verify the vector conservation laws:

$$
\vec{J}=\vec{\ell}+\vec{s} \quad \text { and } \quad \vec{s}=\vec{I}+\vec{i}
$$

where $\vec{I}$ and $\vec{i}$ are the spins of the two particles involved in the collision. The total energy, total angular momentum and parity are conserved during a nuclear reaction. If the model is applied in reverse fashion, i.e. the particle is ejected from the nucleus, the relationship between probabilities of occurrence (cross sections) can be established for both reaction types. This is known as the principle of reciprocity.

### 5.1.3 Principle of Reciprocity

The principle of reciprocity allows the calculation (or at least an estimation) of a reaction cross section as a function of the inverse reaction, as for chemical reactions. (Weinberg and Wigner 1958) cites the example of the ( $\alpha, n$ ) reaction for ${ }_{4}^{9} \mathrm{Be}$ :

$$
\text { Reaction 1: } \quad{ }_{2}^{4} \mathrm{He}+{ }_{4}^{9} \mathrm{Be} \rightarrow{ }_{6}^{12} \mathrm{C}+{ }_{0}^{1} n+Q
$$

the cross section of which is noted as $\sigma_{(\alpha, n)}^{9} B e \quad\left(E_{1}\right)$ with the energy released during the reaction being $Q=5.7 \mathrm{MeV}$. The inverse reaction $(n, \alpha){ }_{6}^{12} C$ is:

$$
\text { Reaction 2: } \quad{ }_{6}^{12} \mathrm{C}+{ }_{0}^{1} n \rightarrow{ }_{2}^{4} \mathrm{He}+{ }_{4}^{9} \mathrm{Be}
$$

with a cross section of $\sigma_{(n, \alpha)}^{{ }_{6}^{6} C}\left(E_{2}\right)$. For a reactive mixture of ${ }_{2}^{4} \mathrm{He},{ }_{4}^{9} B e,{ }_{6}^{12} C$ and ${ }_{0}^{1} n$ at thermal equilibrium, the reaction rates are equal:

$$
v_{1} \sigma_{(\alpha, n)}^{9} B e\left(E_{1}\right)\left[{ }_{4}^{9} B e\right]\left[{ }_{2}^{4} H e\right]=v_{2} \sigma_{(n, \alpha)}^{{ }_{2}^{6} C}\left(E_{2}\right)\left[{ }_{6}^{12} C\right]\left[{ }_{0}^{1} n\right]
$$

At equilibrium, the number of pairs reacting per unit of momentum $d p$ is given by $g p^{2} d p$, i.e. $g p^{2} d E / v$ per unit energy. The coefficient $g$ is a statistical factor that depends on particle spins and it can be computed quite simply in practice. Hence, the reciprocity principle is written as follows:

$$
\frac{\frac{\sigma_{(\alpha, n)}^{9} B e}{\sigma_{1}^{4}}\left(E_{1}\right)}{\sigma_{(n, \alpha)}^{12} C}\left(E_{2}\right) \quad \frac{g_{2}}{\sigma_{1}} \frac{p_{2}^{2}}{p_{1}^{2}}
$$

where $g_{1}=\left(2 I_{{ }_{2}} \mathrm{He}+1\right)\left(2 I_{4} \mathrm{Be}+1\right)$ is the statistical weight of the ${ }_{2}^{4} \mathrm{He}+{ }_{4}^{9} \mathrm{Be}$ pair, $I_{2}^{4} \mathrm{He}$ is the spin of the $\alpha$-particle (here equal to 0 ), and $I_{4}{ }_{4} B e$ that of the ${ }_{4}^{9} \mathrm{Be}$ nucleus (equal to $3 / 2$ ).

$$
p_{1}=\sqrt{2 \mu_{1} E_{1}}=\sqrt{2 \frac{m_{2}^{4} \mathrm{He} m_{4}^{9} \mathrm{Be}}{m_{2}^{4} \mathrm{He}+m_{4} \mathrm{Be}} E_{1}}
$$

is the momentum in the center-of-mass frame for reaction 1. $g_{2}=\left(2 I_{11_{6} C}+1\right)$ $\left(2 I_{0^{n} n}+1\right)$ is the statistical weight of the ${ }_{6}^{12} C+{ }_{0}^{1} n$ pair, with $I_{6}^{12} C$ being the spin of the ${ }_{6}^{12} C$ nucleus and $I_{0^{1} n}$ that of the neutron (equal to $1 / 2$ ).

Similarly: $\quad p_{2}=\sqrt{2 \mu_{2} E_{2}}=\sqrt{2 \frac{m_{12} c^{m_{0}^{1} n}}{m_{12} c^{2}+m_{0}^{1}} E_{2}}$ is the momentum in the center of mass frame for reaction 2 . The energies are related to each other through reaction energy $E_{2}=E_{1}+Q$. The principle of reciprocity is particularly useful in estimating cross sections for "exotic" reactions where no measurement is available for the most usual inverse reaction; for instance the photon-neutron reaction $(\gamma, n)$ is described from the capture cross section $(n, \gamma)$, which is often better known.

### 5.2 Single-Level Breit-Wigner Formalism

Several cross section formalisms have been developed (Fröhner 2000, p. 54): the Blatt-Biedenharn, the $R$ transfer matrix model of Wigner-Eisenbud (exact model), the $R$-matrix model of Kapur-Peierls (also exact), the Single Level Breit-Wigner (SLBW) formalism (the least precise though most commonly used model), the Multi-Level Breit-Wigner (MLBW) approximation, which extends the latter, the Adler-Adler Multi-Level formalism, and the Multi-Level Reich-Moore formalism, which remains the most precise approximation. Most of these models are outside the scope of this book. Focus will be on the simplest model, the SLBW, which is very satisfactory for most industrial applications or for understanding resonant absorption. In 1936, G. Breit and E. P. Wigner proposed a formalism for modeling cross sections in a multi-level model. ${ }^{4}$ The latter may be simplified into a compound nucleus from a reactive pair, noted 1 (in the present case, a neutron and a target nucleus). The total cross section is given by:

$$
\begin{equation*}
\text { Breit-Wigner Formalism : } \quad \sigma_{1}(E)=\frac{\pi h^{2}}{p_{1}^{2}} \frac{g_{c}}{g_{1}} \frac{\Gamma_{1} \Gamma}{\left(\frac{\Gamma}{2}\right)^{2}+\left(E-E_{0}\right)^{2}} \tag{5.1}
\end{equation*}
$$

where $g_{c}$ is the weight of the compound nucleus ${ }^{5}: g_{c}=2 I_{c}+1$. Since $\quad \Gamma_{2} / \Gamma$ is the probability of generating pair 2 (i.e. channel towards 2 ), the cross section $1 \rightarrow 2$ is written as:

$$
\sigma_{1 \rightarrow 2}(E)=\frac{\pi h^{2}}{p_{1}^{2}} \frac{g_{c}}{g_{1}} \frac{\Gamma_{1} \Gamma_{2}}{\left(\frac{\Gamma}{2}\right)^{2}+\left(E-E_{0}\right)^{2}}=4 \pi \hbar_{1}^{2} g \frac{\frac{\Gamma_{1} \Gamma_{2}}{\Gamma^{2}}}{1+\frac{4\left(E-E_{0}\right)^{2}}{\Gamma^{2}}} \text { with } g \equiv \frac{g_{c}}{g_{1}}
$$

[^84]
### 5.2.1 Total Cross Section

Breit and Wigner established that the total cross section could be written as the sum of a constant energy-independent cross section ${ }^{6}$ (the potential cross section), a symmetrical term with respect to the energy of the resonance, and an interference term between the resonance and the potential diffusion (Progress in Fast Neutron Physics 1963, p. 280) of asymmetric form:

$$
\sigma_{t}(E)=4 \pi R^{2}+4 \pi \hbar^{2} g \frac{\Gamma_{n}}{\Gamma} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}+\sqrt{4 \pi \hbar^{2} g 4 \pi R^{2} g} \frac{\frac{\Gamma_{n}}{\Gamma} 4\left(\frac{E-E_{0}}{\Gamma}\right)}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}
$$

The potential cross section, given by $4 \pi R^{2}$, corresponds in wave mechanics to the interaction of a neutron (wave) with the potential at the nuclear surface. In reality, the neutron does not penetrate the nucleus and no compound nucleus is formed (Kahan and Gauzit 1957; GA volume 1, 1967, p. 114). This potential reflection is also referred to as shape elastic scattering since it depends solely on the shape and the transparency of the target nucleus. It varies slightly with energy (for uranium 238, this cross section is roughly equal to 10.7 barns). The potential scattering cross section characterizes the elastic collision of a "ball" of outer surface area $4 \pi R^{2}$. At low energies, the cross section varies as the inverse of the velocity, and the scattering cross section consists only of its potential contribution. The total cross section is often shown in the more convenient form:

$$
\sigma_{t}(x)=\sigma_{p}+\sigma_{t 0} \frac{1}{1+x^{2}}+\sqrt{\sigma_{t 0} \sigma_{p} g} \sqrt{\frac{\Gamma_{n}}{\Gamma}} \frac{2 x}{1+x^{2}}
$$

where $x_{[-]}=\left(E-E_{0}\right) /(\Gamma / 2)$ is the reduced energy and $\sigma_{p}=4 \pi R^{2}$ is the potential scattering cross section, which corresponds to the surface of the nucleus (assuming that it is in fact a perfect sphere of radius $R$ ), and not the longitudinal cross section of the nucleus ( $=\pi R^{2}$ ).

$$
g \equiv \frac{g_{c}}{g_{1}}=\frac{\left(2 I_{A+1} X^{*}+1\right)}{\left(2 I_{A_{2} X}+1\right)\left(2 I_{0_{n}}+1\right)}=\frac{\left(2 I_{A+1} X^{*}+1\right)}{\left(2 I_{z_{A}} X+1\right) 2} \quad \text { as } \quad I_{0^{1}}=\frac{1}{2}
$$

$I_{A+{ }_{2} X^{*}}$ is the spin of the compound nucleus, $I_{A+{ }_{2} X^{*}}=I_{A_{2} X} \pm 1 / 2$ using the rule for spin combination. $\quad \sigma_{t 0}=4 \pi \hbar^{2} g \Gamma_{n} / \Gamma$ is the value of the total cross section at the resonance peak, and depends on energy as follows:

[^85]$$
\Gamma_{n}(E)=\Gamma_{n}\left(E_{0}\right) \sqrt{\frac{E}{E_{0}}} \quad \text { and } \quad \lambda^{2}=\frac{h^{2}}{p^{2}}=\frac{h^{2}}{2 \mu E}
$$

Finally: $\quad \sigma_{t}(E)=\sigma_{p}+\sigma_{t 0} \frac{1}{1+x^{2}}+\sigma_{t 0} \frac{R}{\lambda} \frac{2 x}{1+x^{2}}$

### 5.2.2 Scattering Cross Section

The scattering cross section (i.e. $\Gamma_{1}=\Gamma_{2}=\Gamma_{n}$ in the initial formalism) of neutrons of zero magnetic momentum (which is the case for most neutrons inside a reactor at thermal energy) consists of the potential cross section (optical cross section) and an interference term. It may be written in the following form:

Breit-Wigner scattering cross section :

$$
\begin{align*}
& \sigma_{s}(E)=\underbrace{4 \pi R^{2}}_{\sigma_{p}}+\underbrace{4 \pi \AA^{2} g \frac{\Gamma_{n}}{\Gamma}}_{\sigma_{t 0}} \frac{\frac{\Gamma_{n}}{\Gamma}}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}+\sqrt{\sigma_{t 0} \sigma_{p} g} \sqrt{\frac{\Gamma_{n}}{\Gamma} \frac{\Gamma_{n}}{\Gamma} 4\left(\frac{E-E_{0}}{\Gamma}\right)} \\
&=\sigma_{p}+\sigma_{t 0} \frac{\Gamma_{n}}{\Gamma} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}} \\
&=\sigma_{p}+\sigma_{s 0} \frac{1}{1+x^{2}}+\sqrt{\sigma_{t 0} \frac{\Gamma_{n}}{\Gamma} \sigma_{p} g} \frac{\Gamma_{n}}{\Gamma} \frac{2 x}{1+x^{2}}  \tag{5.2}\\
& 1+\frac{\Gamma_{n}}{\Gamma} \frac{2 x}{1+x^{2}}
\end{align*}
$$

In references, the scattering cross section is often simplified to:

$$
\sigma_{s}(E)=\sigma_{p}+\sigma_{s 0}(E) \frac{1}{1+x^{2}}+\sqrt{\sigma_{s 0}(E) \sigma_{p} g} \frac{\Gamma_{n}}{\Gamma} \frac{2 x}{1+x^{2}}
$$

where

$$
\sigma_{s 0}(E)=\sigma_{t 0}(E) \frac{\Gamma_{n}}{\Gamma}=4 \pi \AA^{2} g \frac{\Gamma_{n}^{2}}{\Gamma^{2}}
$$

### 5.2.3 Radiative Capture Cross Section

For the radiative capture cross section, the general formalism with $\Gamma_{1}=\Gamma_{n}$ and $\Gamma_{2}=\Gamma_{\gamma}$ is used:

$$
\sigma_{n, \gamma}(E)=\underbrace{4 \pi \AA^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}}}_{\sigma_{n, \gamma} 0} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}=\sigma_{n, \gamma} 0 \frac{1}{1+x^{2}}
$$

where $\quad \sigma_{n, \gamma 0}=\sigma_{t 0}(E) \frac{\Gamma_{\gamma}}{\Gamma}=4 \pi \lambda^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}}$
There is no potential cross section for the capture reaction.
The first resonance at 6.64 eV for ${ }_{92}^{238} U$ is of the utmost importance for reactors in which uranium is the predominant isotope.

Breit-Wigner capture cross section :

$$
\begin{equation*}
\sigma_{n, \gamma}(E)=4 \pi \hbar^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}=\sigma_{n, \gamma} 0 \frac{1}{1+x^{2}} \tag{5.3}
\end{equation*}
$$

For most even-even target nuclei (e.g. ${ }_{92}^{238} U$ ), and $I=0$, hence $g_{j}=1 . \lambda$ is the neutron wavelength:

$$
\lambda=\frac{\hbar}{p}=\frac{\hbar}{\mu \cdot v} \approx \frac{h}{2 \pi m v}
$$

for heavy target nuclei since $m_{\text {neutron }} \ll m_{\text {target }}$.

$$
\lambda^{2}=\frac{h^{2}}{4 \pi^{2} m^{2} v^{2}}=\frac{h^{2}}{8 m \pi^{2}} \cdot \frac{1}{E} \quad \text { as } \quad E=\frac{1}{2} m v^{2}
$$

Basic nuclear data: $\Gamma=0.0265 \mathrm{eV}, g=1, \Gamma_{n}=0.00148 \mathrm{eV}, \Gamma_{\gamma}=0.025 \mathrm{eV}$, $E_{0}=6.64 \mathrm{eV}$ in the center-of-mass frame ( 6.67 eV in the laboratory frame).

$$
\begin{gathered}
\sigma_{t}\left(E_{0}\right)=4 \pi \cdot \lambda^{2} \cdot \frac{\Gamma_{n}}{\Gamma}=\frac{h^{2}}{2 \pi m \cdot E_{0}} \frac{\Gamma_{n}}{\Gamma} \\
\sigma_{t}\left(E_{0}\right)=\frac{\left(6.62 .10^{-34}[\mathrm{~J} . \mathrm{s}]\right)^{2}}{2 \times 3.14 \times 1,67.10^{-27}[\mathrm{Kg}] \times 6.64[\mathrm{eV}] \times 1.6 .10^{-19}\left[\mathrm{~J} . \mathrm{eV}{ }^{-1}\right]} \cdot \frac{0.00148[\mathrm{eV}]}{0.0265[\mathrm{eV}]} \\
\sigma_{t}\left(E_{0}\right)=2.1956 .10^{-24}\left[\frac{\mathrm{~J} . \mathrm{s}^{2}}{K g}\right]=2.195610^{+4} \cdot\left[10^{-24} \mathrm{~cm}^{2}\right]=21956 \text { barns } \\
\sigma_{n, \gamma 0}=\sigma_{t 0}(E) \frac{\Gamma_{\gamma}}{\Gamma}=21956 \frac{0.025}{0.0265}=20713 \text { barns } \\
\sigma_{n, \gamma}(E)=\underbrace{4 \pi \lambda^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}}}_{\sigma_{n, \gamma}} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}=\sigma_{n, \gamma 0} \frac{1}{1+x^{2}}
\end{gathered}
$$

### 5.2.4 Fission Cross Section

For fission cross sections, the general equation is used with $\Gamma_{1}=\Gamma_{n}$ and $\Gamma_{2}=\Gamma_{f}$ :
Breit-Wigner fission cross section :

$$
\begin{equation*}
\sigma_{f}(E)=\underbrace{4 \pi \lambda^{2} g \frac{\Gamma_{n} \Gamma_{f}}{\Gamma^{2}}}_{\sigma_{n, \gamma} 0} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}=\sigma_{f 0} \frac{1}{1+x^{2}} \tag{5.4}
\end{equation*}
$$

with $\quad \sigma_{f 0}=\sigma_{t 0}(E) \frac{\Gamma_{f}}{\Gamma}=4 \pi \lambda^{2} g \frac{\Gamma_{n} \Gamma_{f}}{\Gamma^{2}}$

### 5.2.5 Absorption Cross Section

If the two main channels by which neutrons are lost, i.e. the fission and capture cross sections, are added, the absorption cross section is obtained as follows:

$$
\begin{aligned}
\sigma_{a}(E) & =\sigma_{n, \gamma}(E)+\sigma_{f}(E) \\
& =\underbrace{4 \pi \AA^{2} g \frac{\Gamma_{n}\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{\Gamma^{2}}}_{\sigma_{a 0}} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}}=\sigma_{a 0} \frac{1}{1+x^{2}}
\end{aligned}
$$

The $1 / v$ behavior is obtained at low energies, where only neutrons of orbital angular momentum $\ell=0$ interact to form the compound nucleus. In this process, it is assumed that $\lambda \sim 1 / \sqrt{E}, \Gamma_{n, \ell}=\Gamma_{n, 0}^{0} V_{\ell} \sqrt{E}$, where $V_{\ell}$ is called the penetrating factor, $\sigma_{p} \sim c s t$ and $\Gamma_{\gamma} \sim c s t$. Far from the resonances, the distance of $E-E_{0}$, if larger than 1 eV , is predominant over the resonance width $\Gamma$, which is generally only a few thousandths of an eV . At very low energies where $E \ll E_{0}$, the cross section may be simplified as follows:

$$
\sigma_{\gamma}(E) \sim \pi \underbrace{\frac{1}{E}}_{\boldsymbol{\hbar}^{2}} g \frac{\sqrt{E} c s t}{\left(E-E_{0}\right)^{2}+\underbrace{c s t}_{\left({ }^{T_{i}} / 2\right)^{2}}}
$$

Thus, the cross section is inversely proportional to the square root of the energy:

$$
\sigma_{\gamma}(E) \sim \frac{1}{\sqrt{E}}
$$

This relation has been confirmed experimentally. It is particularly well verified for the ( $n, \alpha$ ) cross section of ${ }_{5}^{10} B$ over the whole energy spectrum of nuclear reactors.

### 5.2.6 Negative Resonances

Although possibly surprising, cross sections may have negative resonances. The latter correspond to energy levels that cannot be reached by the capture of a neutron. The negative levels of these bound states are computed using theoretical models. Yet the "wings" of these "fictitious" resonances influence the shape of the cross section at low energy when the "mirror" energy of the first bound state is closer to the neutron-target threshold reaction than to the first non-bound state $\left(\left|E_{0}\right|<E_{1}\right)$. The asymptotic tendency in the vicinity of a negative resonance $E_{0}<0$ is the same as for a positive resonance of a non-bound state for the "mirror" energy of $I E_{0} \mid$. Far to the right of the resonance, the capture cross section is inversely proportional to $E^{5 / 2}$, i.e. a line of gradient $-5 / 2$ on a logarithmic scale.

$$
\sigma_{n, \gamma}(E)=4 \pi \lambda^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}} \frac{1}{1+4\left(\frac{E-E_{0}}{\Gamma}\right)^{2}} \sim \sqrt{\frac{E_{0}}{E}} \frac{1}{E^{2}} \propto \frac{1}{E^{\frac{5}{2}}}
$$

Figure 5.2 shows the plot of the tendency of a positive resonance ( $E_{0}>0$, upper curve) and a negative resonance ( $E_{0}<0$, lower curve) as a function of the normalized energy (normalized to the modulus of the resonance energy). Both tend towards a $1 / v$ law on the left and a $1 / E^{5 / 2}$ law on the right. Only the tendency close to the resonance itself is different. For a positive resonance, the curve varies as $1 /\left(1+x^{2}\right)$, whereas for the negative resonance, the tendency is regular between the two asymptotes.

### 5.2.7 Distribution of Resonances

Unfortunately, up to now, no model can perfectly predict the precise position and width of resonances, especially in the unresolved range. Nevertheless, Eugen Wigner showed (Weinberg and Wigner 1958; Foderaro 1971, p. 283), that the spacing between levels, $D(E)$, i.e. the interval between two resonances for a given spin, depending on the energy of resonances, follows an empirical fluctuation law of the following form:

Fig. 5.2 Normalized representation of the tendency of the cross section in the neighborhood of a resonance [adapted from (Fröhner 2000, p. 71)]


$$
P(x)=\frac{\pi}{2} x e^{-\frac{\pi}{4} x^{2}} \quad \text { with }: \quad x=\frac{D}{\langle D\rangle}
$$

When computed exactly under the hypothesis of random distribution of resonance energies of the compound nucleus, this law provides a satisfactory approximation at low energy. The partial widths ${ }^{7}$ are correctly described by a statistical $\chi^{2}$ (v) law where $v$ is the number of degrees of freedom, i.e. the final number of output channels for a given reaction ${ }^{8}$ :

$$
P(x, v)=\frac{v}{2 \Gamma\left(\frac{v}{2}\right)}\left(\frac{v x}{2}\right)^{\frac{v}{2}-1} e^{-\frac{v x}{2}}
$$

which includes the real factorial, known as the gamma function: $\Gamma(v / 2)=$ $\int_{0}^{+\infty} t^{\frac{\nu}{2}-1} e^{-t} d t$ and where $x=\Gamma_{i} /\left\langle\Gamma_{i}\right\rangle$ is the reduced resonance width, normalized

[^86]to the mean value. In the case of elastic scattering, the neutron widths $\Gamma_{n}^{0}$ fluctuate significantly between the resonances; since $v=1$ (at low energy, the only output channel with emission of a scattered neutron is the formation channel, and there is thus only one degree of freedom), the Porter-Thomas law ${ }^{9}$ applies:

Porter-Thomas distribution of neutron widths :

$$
\begin{equation*}
P_{\text {Porter-Thomas }}(x) \equiv \frac{1}{\sqrt{2 \pi}} \frac{1}{\sqrt{x}} e^{-\frac{x}{2}} \tag{5.5}
\end{equation*}
$$

In the case of radiative capture, there are very many degrees of freedom, corresponding to the many possible excitation states of the target nucleus, and thus of radiative transitions. In this case $v \gg 1$ and the $\chi^{2}(v)$ law tends towards a Dirac $\delta$ function. The fluctuations of the radiative capture widths are thus very slight and the following approximation is acceptable: $\Gamma_{\gamma}=\left\langle\Gamma_{\gamma}\right\rangle$. With fission, for a given output channel, the fission widths experimentally obey Porter-Thomas distribution with $v \approx 2$ or 3 . Where several exit channels exist $(v>1)$, there are two possibilities:

- either the partial widths $\Gamma_{f_{i}}$ for the fission channels have the same mean value, in which case $\Gamma_{f}$ obeys a $\chi^{2}(v)$ law with $v$ between 1 and 4 (very often 2 ) for the usual fissile isotopes,
- or the mean values are different, in which case, a convolution of several PorterThomas laws should be done.

A statistical resonance in the unresolved range may be defined by taking a random real number in the $[0,1]$ interval and then computing $\gamma=\Gamma_{i} /\left\langle\Gamma_{i}\right\rangle$ by solving the following transcendental equation:

$$
\begin{aligned}
& \int_{0}^{\tau} P_{\text {Porter-Thomas }}(x) d x=\int_{0}^{\gamma} P(x, v) d x \quad \text { i.e. : } \\
& \quad \tau=\frac{1}{\Gamma\left(\frac{v}{2}\right)} \int_{0}^{\gamma}\left(\frac{v}{2} t\right)^{\frac{v}{2}-1} e^{-\frac{v}{2} t} d t=\Gamma\left(\frac{v}{2} \gamma, \frac{v}{2}\right)
\end{aligned}
$$

where an incomplete gamma function is present:

$$
\Gamma(x, \beta)=\frac{1}{\Gamma(\beta)} \int_{0}^{x} t^{\beta-1} e^{-t} d t
$$

[^87]In the case of a single degree of freedom $(v=1)$, the incomplete gamma function degenerates into:

$$
\tau=\operatorname{erf}\left(\sqrt{\frac{\gamma}{2}}\right)
$$

The standard deviation with respect to 1 of $\Gamma_{i} /\left\langle\Gamma_{i}\right\rangle$ is $2 / v_{i}$, i.e. if the number of degrees of freedom is small, as in scattering or fission, the variation in resonance width will be significant from one resonance to another. The larger the number of degrees of freedom, as in neutron capture, the more $\Gamma_{i}$ may be considered to be constant (Foderaro 1971, p. 284).

### 5.2.8 Resonant Absorption

(Dresner 1960; Progress in nuclear energy 1958, Vol 2, p. 233)
For a resonant trap with lethargy of width $\Gamma$ where absorption is infinite (black trap) and zero outside (Fig. 5.3).

As seen in the previous chapter, the probability of escaping a trap (with the entrance of the trap as the origin of lethargies), i.e. the resonance escape probability, is calculated as follows:

$$
\begin{equation*}
\text { Resonance escape probability : } \quad p=\int_{0}^{\Gamma} d u \int_{u-\varepsilon}^{0} \frac{1}{\xi} \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} d u^{\prime} \tag{5.6}
\end{equation*}
$$

The probability of being absorbed in a trap is:


Fig. 5.3 The "kangaroo" neutron with respect to lethargy (Paul Reuss compares the neutron to a carefree kangaroo jumping around in the Australian bush, unaware of possible traps (Reuss 2003, p. 194). These traps represent resonances and are like deep holes from which the kangaroo-neutron cannot escape. However, the kangaroo may jump over a trap without noticing it if it does not land straight in the trap. A "grey" trap is less deep and the neutron may statistically survive. A "black" trap spells the "death" of the neutron by absorption. Hence, the discontinuous slowing-down mechanism allows neutrons to survive in the resonance zone.)

$$
1-p=\frac{1-e^{-\Gamma}-\alpha^{\Gamma}}{\xi(1-\alpha)} \quad \text { if } \Gamma \ll 1, \quad 1-p \approx \frac{\Gamma}{\xi}
$$

G. Placzek showed that the scattering density $R_{s}(u)$ before the trap has an asymptotic value of $1 / \xi$. The value $\Gamma / \xi$ proves that the arrival density in the trap is the same as in the absence of a trap (only the neutrons scattered from the trap to within it are missing, but these are few since $\Gamma$ is small). The resonance escape probability $p$ for a "grey" (low absorption $\Sigma_{a}$ ) but very narrow trap (the $d u / \xi$ neutrons coming from the $d u$ in the trap have a probability of being absorbed of $\Sigma_{a} / \Sigma_{t}$ ) may be deduced by computing the number of neutrons absorbed in the trap:

$$
1-p \approx \int_{0}^{\gamma} \frac{1}{\xi} \frac{\Sigma_{a}(u)}{\Sigma_{t}(u)} d u
$$

For a series of consecutive traps (Stacey 2001, p. 117; Etherington 1957, pp. 6-80), the resonance escape probability factor is written as:

$$
p \approx \prod_{i} p_{i} \approx e^{\left(-\sum_{i} \int_{i} \frac{\Sigma_{a}(u)}{\xi \Sigma_{t}(u)} d u\right)}=e^{-\int_{0}^{u_{\max }} \frac{\Sigma_{a}(u)}{\xi \Sigma_{t}(u)} d u}
$$

Using this formalism, the escape factor in homogeneous situations can be obtained.

### 5.3 Self-Shielding

The very existence of resonances leads to a phenomenon whereby the flux spectrum $\Phi(E)$ in their vicinity is depressed. ${ }^{10}$ The energy flux decreases at the locations of the resonances and thus fewer neutrons are lost than might be expected if the flux were not depressed. This phenomenon is known as self-shielding:

$$
\Phi(E)=\frac{R_{t}(E)}{\Sigma_{t}}=\frac{R_{s}(E)}{\Sigma_{s}} \underset{\begin{array}{c}
\text { Wigner } \\
\text { approximation }
\end{array}}{\approx} \frac{q(E)}{\xi\left(\Sigma_{a}+\Sigma_{s}\right) E}
$$

where $q(E)=E R_{s}(E)=R_{s}(u)$.
In the resonance $\Sigma_{a} \gg \Sigma_{s}$, the absorption rate is thus less significant than if there were no flux $\Phi(E)$ depression (Fig. 5.4). Hence, $\Sigma_{a}(E)$ increases while $\Phi(E)$ decreases such that $\Sigma_{a}(E) \Phi(E)$ remains (relatively) small. This concept is described

[^88]

Fig. 5.4 Self-shielding of a resonance


Fig. 5.5 Self-shielding of the flux owing to the resonances
formally with the use of effective cross sections, defined such as to conserve the reaction rate while keeping the asymptotic flux $\Psi$ (before the resonance).

$$
\Sigma_{a}^{e f f e c t i v e}(u) \Psi=\Sigma_{a}(u) \Phi(u)
$$

Outside the resonances, the cross section consists of the potential cross section only:

$$
\Sigma_{t}(u) \Phi(u) \approx C s t e=\Sigma_{p} \Psi
$$

hence: $\Sigma_{a}^{\text {eff }}(u)=\Sigma_{a}(u) \frac{\Phi(u)}{\Psi}=\Sigma_{a}(u) \frac{\Sigma_{p}}{\Sigma_{t}(u)}$
The coefficient $\frac{\Sigma_{p}}{\Sigma_{t}(u)}$ is called the self-shielding factor (Fig. 5.5).
Furthermore, the effective microscopic cross section is defined as:

$$
\Sigma_{a}^{e f f} \equiv N_{U} \sigma_{a}^{e f f}
$$

where $N_{U}$ is the concentration of the resonant isotope. The effective resonance integral is defined for a given resonance as the integral of the effective cross section over lethargy such that the absorption rate is verified for the asymptotic flux (flux outside the resonance) (Dresner 1960, p. 62):

$$
\int_{\text {resonance }} N_{U} \sigma_{a}^{e f f}(u) \Psi(u) d u \equiv \int_{\text {resonance }} N_{U} \sigma_{a}(u) \Phi(u) d u=\delta q_{\text {res }}
$$

$\delta q_{r e s}$ is the variation in slowing-down density due to the presence of the resonance.
Using $I_{\text {eff, res }} \equiv \int_{\text {resonance }} \sigma_{a}^{\text {eff }}(u) d u$, we obtain the following:

$$
I_{\text {eff, rés }}=\int_{\text {resonance }} \sigma_{a}(u) \frac{\Sigma_{p}}{\Sigma_{t}(u)} d u
$$

and, thus for a set of narrow resonances well spaced in energy: $I_{e f f}=\sum_{r e s} I_{e f f, r e s}=\int_{u} \sigma_{a}(u) \frac{\Sigma_{p}}{\Sigma_{t}(u)} d u$. This enables calculation of the escape probability, which is the product of the escape probabilities for each resonance in a homogeneous case:

$$
p=e^{-\frac{\left(N_{U} I_{\text {eff }}\right)}{\left(\xi \Sigma_{S} S_{\text {moderator }}\right.}}
$$

In the heterogeneous case, it is assumed that the cell consists of the fuel rod surrounded by moderator. Slowing-down is effective only in the moderator and outside the resonances. Therefore, the asymptotic flux is evaluated as follows, where $M$ is the index for the moderator:

$$
\Psi(r, u)=\frac{Q}{\xi \Sigma_{s, M} V_{M}}
$$

$Q$ is the volume integral of the slowing-down density over the cell. As for the homogeneous case, the effective integral is defined by integration over lethargy and fuel volume $V_{U}$ :

$$
\begin{aligned}
\int_{V_{U}} d^{3} r \int_{\text {resonance }} N_{U} \sigma_{a}^{e f f}(u) \Psi(u) d u & =N_{U} V_{U} I_{e f f, \text { res }} \Psi \\
& \equiv \int_{V_{U}} d^{3} r \int_{\text {resonance }} N_{U} \sigma_{a}(u) \Phi(r, u) d u
\end{aligned}
$$

giving: $I_{e f f, r e s} \equiv \frac{1}{V_{U}} \int_{V_{U}} d^{3} r \int_{\text {resonance }} \sigma_{a}(u) \frac{\Phi(r, u)}{\Psi(u)} d u, I_{e f f}=\sum_{r e s} I_{\text {eff }, \text { res }}$ and the heterogeneous escape probability is thus:

$$
p=e^{-\frac{V_{U} N_{U} I_{e f f}}{V_{m} N_{m}\left(\xi \sigma_{S}\right)_{M}}}
$$

### 5.4 Slowing-Down Through Resonances

Let us consider a medium consisting of a mixture of a resonant nuclide (termed $c$ for fuel) and a light nuclide (termed $m$ for moderator). The slowing-down equation is given by the neutron balance at lethargy $u$ without the fission spectrum:

| Arrivals |  |  |
| :--- | :--- | :--- |
| $R_{c}(u)=R_{c}\left[\Sigma_{s}^{c} \Phi\right]=\int_{u-\varepsilon_{c}}^{u} \Sigma_{s}^{c}\left(u^{\prime} \rightarrow u\right)$ | $\Phi\left(u^{\prime}\right) d u^{\prime}$ | Neutrons arriving from energy $u^{\prime}<u$ <br> and scattered at lethargy $u$ by collision <br> over the heavy nuclides. This is <br> expressed by the notation $[$ which <br> introduces the concept of the operator. |
| $R_{m}(u)=R_{m}\left[\Sigma_{s}^{m} \Phi\right]=\int_{u-\varepsilon_{m}}^{u} \Sigma_{s}^{m}\left(u^{\prime} \rightarrow u\right)$ | $\Phi\left(u^{\prime}\right) d u^{\prime}$ | Idem for the light moderator. |
| Departures | Neutrons lost either by absorption or by <br> scattering at another lethargy value |  |
| $\Sigma_{t}^{c}(u) \Phi(u)+\Sigma_{t}^{m}(u) \Phi(u)$ |  |  |

Hence, the slowing-down equation is:

$$
\begin{equation*}
\text { Slowing-down equation : } \quad R_{c}(u)+R_{m}(u)=\Sigma_{t}(u) \Phi(u) \tag{5.7}
\end{equation*}
$$

where
$\Sigma_{t}=\Sigma_{t}^{c}+\Sigma_{t}^{m}$ Total cross section of the medium
$R_{i}(u)=R_{i}\left[\Sigma_{s}^{i} \Phi\right]=\int_{u-\varepsilon_{i}}^{u} \Sigma_{s}^{i}\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime}$ Arrival density due to scattering (slowing down) for material $i$
$\varepsilon_{i}=\log \left(\frac{1}{\alpha_{i}}\right)$ Maximum gain in lethargy per collision on isotope $i$ of material $i$ $\alpha_{i}=\left(\frac{A_{i}-1}{A_{i}+1}\right)^{2}$ Minimum ratio of energy per collision with $A$-ratio of the mass of isotope $i$ to that of the neutron
$\Sigma_{s}\left(u^{\prime} \rightarrow u\right)=\Sigma_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right)$ Differential scattering cross section for isotope $i$
$P\left(u^{\prime} \rightarrow u\right)=\frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha}$ Scattering cross section from $u^{\prime}$ to $u$ if the collision is elastic and isotropic in the center of mass

Physically, it makes sense to consider that $R_{c}(u) \ll R_{m}(u)$ since light nuclides are more efficient for slowing-down. The slowing-down operator for the moderator is said to be "long-range" (lethargy-wise).

Fig. 5.6 Variation of $\Sigma_{t}(u)$ and $\Phi(u)$


Further, it may be assumed that $\rho_{1}(u)$ varies slowly with lethargy since the maximum gain in lethargy $\varepsilon_{1}$, which is very high for light nuclides, is greater than the width of the resonances of heavy isotopes $\Gamma$.

It may thus be concluded that $\Sigma_{t}(u) \Phi(u)$ varies very slowly with lethargy (Fig. 5.6), thus implying that the flux is strongly depressed in the resonance since it follows a $1 / \Sigma_{t}(u) \quad$ law. This flux is called the Bondarenko ${ }^{11}$ spectrum, which characterizes the

[^89]
(Public domain)
flux shape in the resonance. Self-shielding is thus important only if the concentration of the heavy nuclide is not too small (i.e. where dilution is not infinite). Two numerical considerations are possible: either with a very refined energy mesh taking exact account of the variations of $\Sigma$, and thus of $\Phi$, as a function of $u$, which leads to thousands of groups and thus involves long calculation times in daily use; or else a simplified model can be set up to allow the use of a coarser energy mesh for precise calculation. The latter ${ }^{12}$ is used in the Livolant-Jeanpierre formalism (1969). ${ }^{13}$

[^90]

Alain Santamarina in 2011 (Courtesy Santamarina)
${ }^{13}$ Michel Livolant (b. 1938). After his studies at the Ecole Polytechnique, he completed the second Master's degree course in reactor physics to be given at Saclay in 1963. His original theoretical works are on self-shielding theory. His rapid career path at $C E A$ saw him nominated head of the "Institut de Protection et de Sûreté Nucléaire", which would later become the IRSN.

Françoise Jeanpierre-Gantenbein (b. 1944) obtained her PhD in physics in 1969 after a BSc in physics at University of Orsay (1966) and a Master's in reactor physics in 1967. She began her career at the CEA/Service de Physique Mathématique at Saclay from 1967 to 1971. Later, she worked on seismic mechanics. From 1988 to 1995, she was head of the Seismic Studies laboratory where the European TAMARIS facility is located. She became a senior expert in seismic questions at $C E A$. She coordinated research programs in safety from 1998 until retiring in 2007.

Photo 5.3 Michel Livolant (b. 1938) (Courtesy

Livolant)


Photo 5.4 Françoise
Jeanpierre (b. 1944)
(Courtesy Jeanpierre)


### 5.5 The Livolant-Jeanpierre Formalism

### 5.5.1 Homogeneous Medium

Let us consider the simple case of a homogeneous medium consisting of a resonant isotope ( $c$ is the fuel index, stands for combustible in French) of concentration $N_{c}$ with total macroscopic cross section $\Sigma_{t}^{c}$ and a moderator of total cross section $\Sigma_{t}^{m}\left(\Sigma_{a}^{m} \approx 0\right)$. Assuming that $\Sigma_{t}^{m}$ is constant or varies slowly with energy, ${ }^{14}$ the neutron slowing-down balance at lethargy $u$ is written as:

[^91]\[

$$
\begin{aligned}
& \int_{u-\varepsilon_{c}}^{u} \Sigma_{s}^{c}\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime}+\int_{u-\varepsilon_{m}}^{u} \Sigma_{s}^{m}\left(u^{\prime} \rightarrow u\right) \quad \Phi\left(u^{\prime}\right) d u^{\prime} \\
& =\Sigma_{t}^{c}(u) \Phi(u)+\Sigma_{t}^{m}(u) \Phi(u)
\end{aligned}
$$
\]



The technical report CEA-R-4533 (1974) which stems from the original works of LivolantJeanpierre (The Marguet collection) (Photo 5.3)


Jules Horowitz's personal copy of Françoise Jeanpierre's doctoral thesis (September 1969) (The Marguet collection) (Photo 5.4)

Let $R$ be the slowing-down operator (in brackets), applied to the flux:

$$
R[]=\int_{u-\varepsilon}^{u} \Sigma_{s}\left(u^{\prime} \rightarrow u\right)[] d u^{\prime}
$$

The equation is then written in the following form:

$$
R_{c}[\Phi]+R_{m}[\Phi]=\left(\Sigma_{t}^{c}(u)+\Sigma_{t}^{m}(u)\right) \Phi(u) \approx\left(\Sigma_{t}^{c}(u)+\Sigma_{s}^{m}\right) \Phi(u)
$$



Fig. 5.7 Decomposition of flux into macroscopic flux and fine structure flux

From now on, the reader should be aware that $R$ is an operator and that $R[\Phi]$ is not a multiplication but the application of the operator to the flux inside the brackets. Since the flux varies as $1 / E$, it should be noted that it is constant in lethargy as prescribed in the Wigner model (without absorption). The true flux varies slowly with lethargy owing to absorptions. Some approximations are applied to solve the slowing-down equation with "large" energy groups (since few energy groups are used in industrial calculations). The real flux, $\Phi$, is factorized in an asymptotic macroscopic term $\Psi$ (which has the unit dimensions of the flux) and a second component, called fine structure, $\varphi$ (dimensionless, usually called fine flux), which is constant outside the resonances: $\Phi=\Psi \varphi$ (Fig. 5.7).

### 5.5.2 Fine Structure Equation

The slowing-down operator for a heavy nuclide is applied over a very small lethargy range, $\varepsilon_{c}$ (about 0.02 for ${ }^{238} U$ ). It is assumed that $\Psi$ does not vary significantly over $\varepsilon_{c}$.

$$
R_{c}[\Phi]=R_{c}[\Psi \varphi] \approx \Psi R_{c}[\varphi]
$$

The narrow resonance approximation is applied to the slowing-down operator for the moderator, i.e. $R_{m}[\Phi] \approx \Sigma_{s}^{m} \Psi$. The term cancels out on both sides of the slowing-down equation, and the resulting equation is the fine structure equation, which describes the energy coupling:

Homogeneous fine structure equation : $\frac{1}{N_{c}} R_{c}[\varphi]+\frac{\Sigma_{s}^{m}}{N_{c}}=\left(\sigma_{t}^{c}(u)+\frac{\Sigma_{t}^{m}}{N_{c}}\right) \varphi(u)$

The microscopic operator is defined as $r_{c}[] \equiv R_{c}[] / N_{c}$ (using the analogy with microscopic cross sections). The equivalent microscopic cross section $\sigma_{e} \equiv \Sigma_{s}^{m} / N_{c}$, also called the dilution cross section or simply dilution, is more or
less independent of lethargy, but depends on the moderator via $\Sigma_{s}^{m}$ and on the resonant isotope via $N_{c}$. The fine structure equation $\varphi$ is independent of $\Sigma_{t}^{c}$ and $N_{m}$ :

$$
r_{c}[\varphi]-\left(\sigma_{t}^{c}(u)+\sigma_{e}\right) \varphi(u)+\sigma_{e}=0
$$

In this expression, $\varphi$ is a function of $\sigma_{e}$, which depends on the total macroscopic cross section of the slowing-down (moderator) isotope and the concentration of the resonant isotope. The equivalent cross section in a homogeneous medium can hence be assumed to be independent of lethargy. Therefore, in a homogeneous medium, the fine structure equation can be solved accurately for a few values of $\sigma_{e}$ and temperature $T$ using a refined energy mesh (several thousand groups). In France, this resolution is done historically using a dedicated software called AUTOSECOL, which solves a purely slowing-down problem. The effective cross sections per energy group $g$ for a reaction $r$ and the resonant isotope are given by:

$$
\begin{aligned}
& \sigma_{r, e f f}^{c, g}=\frac{1}{\int_{u_{g}}^{u_{g}+\Delta u_{g}} \varphi(u) d u} \int_{u_{g}}^{u_{g}+\Delta u_{g}} \sigma_{r}^{c}(u) \varphi(u) d u \\
& =\frac{1}{\Delta u_{g}} \int_{u_{g}}^{u_{g}+\Delta u_{g}} \sigma_{r}^{c}(u) \varphi(u) d u
\end{aligned}
$$

since $\varphi(u)=1$ except in the resonances. The cross sections $\sigma_{r, e f f}^{c, g}$ are tabulated as a function of the dilution $\sigma_{e}$ (effective absorption, scattering, and production cross sections) and of $T$. Applying the Narrow Resonance ( $N R$ ) hypothesis (which is described in the next paragraph ${ }^{15}$ ) to the slowing-down operator for heavy nuclides enables analytical calculation of the fine structure using:

$$
\left\{\begin{array}{l}
r_{c}\left[\varphi^{N R}\right]=\sigma_{p} \\
\varphi^{N R}(u)=\frac{\sigma_{p}+\sigma_{e}}{\sigma_{t}^{c}(u)+\sigma_{e}}
\end{array}\right.
$$

Using the Wide Resonance (WR) hypothesis, the fine structure is:

$$
\left\{\begin{array}{l}
r_{c}\left[\Sigma_{s}^{c} \varphi^{W R}\right]=\Sigma_{s}^{c}(u) \varphi^{W R}(u) \text { hence } \frac{1}{N_{c}} \Sigma_{s}^{c}(u) \varphi^{W R}(u)+\frac{\Sigma_{s}^{m}}{N_{c}}=\left(\sigma_{t}^{c}(u)+\frac{\Sigma_{t}^{m}}{N_{c}}\right) \varphi^{W R}(u) \\
\varphi^{W R}(u)=\frac{\frac{\Sigma_{s}^{m}}{N_{c}}}{\sigma_{a}^{c}(u)+\frac{\Sigma_{t}^{m}}{N_{c}}}=\frac{\sigma_{e}}{\sigma_{a}^{c}(u)+\frac{\Sigma_{t}^{m}}{\Sigma_{s}^{m}} \sigma_{e}}
\end{array}\right.
$$

[^92]
### 5.5.3 Tabulating Effective Cross Sections

The reaction rate over the lethargy range $\left[u_{g}, u_{g+1}\right]$ is defined as:

$$
T_{r}=\int_{u_{g}}^{u_{g+1}} \sigma_{r}(u) \Phi(u) d u=\Phi_{g} \sigma_{r}^{g} \Delta u_{g}
$$

where $g$ lethargy group corresponding to $\left[u_{g}, u_{g+1}\right]$
$\sigma_{r}$ microscopic cross section for reaction $r$
The flux is factorized as $\Phi(u)=\Psi(u) \phi(u)$. Supposing that the macroscopic component $\Psi(u)$ decays slowly over the interval $\left[u_{g}, u_{g+1}\right]$ (which is the case for heavy nuclides in thermal reactors when using energy meshes with approximately 200 groups as used by APOLLO2 spectral code), the calculation of the reaction rate:

$$
T_{r}=\bar{\Psi} \int_{u_{g}}^{u_{g+1}} \sigma_{r}(u) \varphi(u) d u \quad \text { with } \bar{\Psi}=\Psi\left(\frac{u_{g}+u_{g+1}}{2}\right)
$$

The effective cross section is described as:

$$
\sigma_{e f f}^{g} \equiv \frac{1}{u_{g+1}-u_{g}} \int_{u_{g}}^{u_{g+1}} \sigma_{r}(u) \varphi(u) d u
$$

This cross section takes into account variation in fine structure $\varphi(u)$ for the cross section $\sigma$ over the interval $\left[u_{g}, u_{g+1}\right]$. Integrating over a group $g$ of lethargy width $\Delta u_{g}=u_{g+1}-u_{g}$, the following is obtained:

$$
\left\{\begin{array} { l } 
{ T _ { r } ^ { g } = \overline { \Psi } _ { g } \sigma _ { e f f } ^ { g } \Delta u _ { g } } \\
{ T _ { r } ^ { g } = \Phi _ { g } \sigma _ { r } ^ { g } \Delta u _ { g } }
\end{array} \quad \text { with } \quad \left\{\begin{array}{c}
\sigma_{e f f}^{g}=\sigma_{r}^{g} \varphi_{g} \\
\Phi_{g} \sigma_{r}^{g}=\bar{\Psi}_{g} \sigma_{e f f}^{g}
\end{array}\right.\right.
$$

Thus, the effective cross section enables computation of the correct reaction rate where variation in the macroscopic component of the flux alone is taken into account. This parameter is tabulated in a homogeneous medium. The effective integral $I_{\text {eff }}$ is hence defined as:

$$
I_{e f f} \equiv \int_{u_{0}}^{u_{t h}} \sigma_{r}(u) \varphi(u) d u \equiv \sum_{g \in\left[u_{0}, u_{t h}\right]} \Delta u_{g} \sigma_{r, e f f}^{g}
$$

where:
$u_{0}$ :lethargy corresponding to the maximum useful energy ( 10 MeV );
$u_{t h}$ : lethargy corresponding to a given thermal cut-off.

Henceforth, for a given homogeneous problem, only the dilution of the problem $\sigma_{e} \equiv \Sigma_{s}^{m} / N_{c}$ is required. The effective cross sections by group are obtained directly by interpolation from the table computed for a very fine energy mesh. The fine structure equation is discretized over the multi-group energy mesh of the transport code so as to determine $\varphi_{g}$ for each group. It should be noted that at the boundaries, the fine structure is constant (equal to 1 ), and there is thus no leakage:

$$
\begin{cases}\sum_{g^{\prime}} \sigma_{s}^{c, g^{\prime} \rightarrow g} \varphi_{g^{\prime}}+\sigma_{e}=\left(\sigma_{t}^{c, g}+\sigma_{e}\right) \varphi_{g} & \\ \sum_{g^{\prime}} \sigma_{s, e f f}^{c, s^{\prime} \rightarrow g}+\sigma_{e}=\left(\sigma_{t}^{c, g}+\sigma_{e}\right) \varphi_{g} & \text { with } \quad \sigma_{s, e f f}^{c, g^{\prime} \rightarrow g}=\sigma_{s}^{c, g^{\prime} \rightarrow g} \varphi_{g^{\prime}} \\ \varphi_{g}=1-\frac{\sigma_{t, e f f}^{c, g}}{\sigma_{e}}+\frac{\sum_{g^{\prime}} \sigma_{s, e f f}^{c, g^{\prime} \rightarrow g}}{\sigma_{e}} & \text { with } \quad \sigma_{t, e f f}^{c, g}=\sigma_{t}^{c, g} \varphi_{g}\end{cases}
$$

Hence, the multi-group self-shielded cross sections for reaction $r$ and the resonant isotope (c) are obtained by computing the fine structure of the coarse energy mesh:

$$
\sigma_{r}^{c, g}=\frac{\sigma_{r, e f f}^{c, g}}{\varphi_{g}}
$$

Figure 5.8 sums up the resolution process for a homogeneous problem.


Fig. 5.8 Interpolating as a function of the dilution of the effective cross sections

### 5.6 Modeling the Slowing-Down Operator Using the Resonant Isotope

### 5.6.1 Narrow Resonance Approximation

The slowing-down term $\int_{u-\varepsilon}^{u} \Sigma_{s}\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime}$ can be approximated using a simplified slowing-down model: the narrow resonance ( $N R$ ) approximation (Stacey 2001, p. 118) (Fig. 5.9).

Where the resonance width $\Gamma$ is small compared to the maximum lethargy gain per collision $\varepsilon$, the most important factor in slowing-down is the lethargies, $u^{\prime}$, which are very small compared to lethargy $u$. In this case, the scattering cross section $\Sigma_{s}$ tends towards the potential cross section of the mixture $\Sigma_{p}$ while the flux is equal to its asymptotic value $\Phi_{a s}$ (assuming that the resonances are sufficiently spaced in energy so that the flux between two resonances is asymptotic).

$$
\begin{aligned}
\int_{u-\varepsilon}^{u} \Sigma_{s}\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime} & =\int_{u-\varepsilon}^{u} \Sigma_{s}\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime} \\
& \approx \int_{u-\varepsilon}^{u} \Sigma_{p} P\left(u^{\prime} \rightarrow u\right) \Phi_{a s} d u^{\prime} \\
& =\Sigma_{p} \Phi_{a s} \underbrace{\int_{u-\varepsilon}^{u} \frac{e^{\left(u^{\prime}-u\right)}}{1-\alpha} d u^{\prime}}_{1}
\end{aligned}
$$

thus: $\quad R\left[\Phi^{N R}\right] \approx \Sigma_{p} \Phi_{a s}$
It should be noted that the slowing-down operator becomes independent of the arrival lethargy. The NR approximation is applied to the slowing-down operator:

$$
R_{m}\left[\Phi^{N R}\right]=\Sigma_{s}^{m} \Psi \approx \Sigma_{p} \Phi_{a s}
$$



Fig. 5.9 NR approximation
since $\varphi=1$ outside the resonances and $\Psi=\Phi_{a s}$. Expressed in lethargy, $\Phi_{a s}$ is constant $\left(\Phi_{\text {epi }}\right)$, though in energy, $\Phi_{a s}$ is inversely proportional to energy ( $\left.\Phi_{\text {epi }} / E\right)$. The cross section $\Sigma_{s}^{m}$ has a slow variation as well as $R_{m}[\Phi]$ since the lethargy range $\varepsilon_{m}$ on which integration is carried out is large compared to the resonance widths. The long-energy-range operator $R_{m}$ smoothens the fine structure. Hence, the slowing down due to the light nuclide is not considered. This hypothesis is justified for a homogeneous mixture of water and uranium, where slowing down is caused mainly by the hydrogen in the water. In this case, the maximum gain in lethargy is much more significant than for uranium, except in the unresolved range of ${ }^{238} U$, where the resonances are very close.

However, this hypothesis should be applied cautiously for heavy nuclides, as well as for intermediate-mass nuclides such as oxygen in $\mathrm{UO}_{2}$.

### 5.6.2 Wide Resonance Approximation

The wide resonance (WR) approximation assumes that the maximum gain in lethargy is small compared to the width of the resonance, in which case it may be assumed that the quantities $\Sigma_{s}$ and $\Phi$ vary weakly over that interval (Stacey 2001, p. 119):

$$
R\left[\Phi^{W R}\right] \approx \Sigma_{s}(u) \Phi(u)
$$



The slowing-down operator depends only on the arrival lethargy via the scattering cross section and the flux. The coupling in energy is no longer present.

### 5.6.3 Statistical Approach

The statistical approach of Mireille Coste ${ }^{16}$ (2003) consists in supposing that the resonances of the resonant isotope are narrow and statistically distributed within an energy group. Their spacing, $D$, is considered to be small with respect to the maximum gain in lethargy for the resonant isotope $\varepsilon_{c}$. The slowing-down operator for the heavy nuclide can be substituted by a mean value for the energy group.

$$
\begin{aligned}
R_{c}\left[\Phi^{S T}\right] & =\int_{u-\varepsilon_{c}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) P\left(u^{\prime} \rightarrow u\right) d u^{\prime} \underset{\alpha_{c} \approx 1}{\approx} \frac{1}{\varepsilon_{c}} \int_{u-\varepsilon_{c}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} \\
& \varepsilon_{c} \ll 1 \frac{1}{\Delta u_{g}} \int_{u_{g}}^{u_{g+1}} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime}
\end{aligned}
$$

In fact, the collision law approaches a uniform law where $\alpha_{c} \approx 1$ and where $\varepsilon_{c} \ll 1$, in which case $e^{-\left(u-u^{\prime}\right)} \approx 1$ si $\left(u-u^{\prime}\right)<\varepsilon_{c}$.


The slowing-down operator no longer depends on the arrival lethargy but on a mean value dependent on the energy group. The $S T$ model also works correctly both in the unresolved range and in the high end of the resolved range, where resonances, though narrow, are widespread within an energy group.

[^93]
### 5.6.4 All Resonance Model (TR)

Mireille Coste's All Resonance model (developped in 1997) is a generalization of the ST model that seeks to remove all potential constraints on the shape and position of resonances so as to obtain a "universal" model (Photo 5.5). An energy group is sub-divided into $g$ subgroups defined by (Fig. 5.10):

$$
\left.W\left(g^{\prime}, g\right) \equiv\left\{u \in g / u-\varepsilon_{c} \in g^{\prime}\right\}\right)
$$

By construction, $g^{\prime}$ cannot be larger than $g$ (the groups are numbered along increasing lethargies). The integration range of the slowing-down operator for heavy nuclides (its "reach" or "range") may be expanded as follows:

$$
\begin{aligned}
{\left[u-\varepsilon_{c}, u\right]=} & {\left[u-\varepsilon_{c}, u_{\max }\left(g^{\prime}\right)\right] \cup\left[u_{\min }\left(g^{\prime}+1\right), u_{\max }\left(g^{\prime}+1\right)\right] } \\
& \times \cup\left[u_{\min }\left(g^{\prime}+2\right), u_{\max }\left(g^{\prime}+2\right)\right] \cup \ldots \cup\left[u_{\min }(g-1), u_{\max }(g-1)\right] \\
& \times \cup\left[u_{\min }(g), u\right]
\end{aligned}
$$

where $u_{\text {min }}\left(g^{\prime}\right)$ and $u_{\text {max }}\left(g^{\prime}\right)$ are the lower and upper lethargies of group $g^{\prime}$. The slowing down of the resonant operator can be computed as:

$$
\begin{aligned}
R_{c}\left[\Phi^{T R}\right] & =\frac{1}{\varepsilon_{c}} \int_{u-\varepsilon_{c}}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime} \\
& =\frac{1}{\varepsilon_{c}}\left[\begin{array}{l}
\left.\int_{u-\varepsilon_{c}}^{u_{\max }\left(g^{\prime}\right)} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime}+\sum_{g^{\prime \prime}=g^{\prime}+1}^{g_{u_{\min }\left(g^{\prime \prime}\right)}^{u}=g-1} \sum_{s}^{u_{\max }\left(g^{\prime \prime}\right)} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime}\right] \\
+\int_{u_{\min }(g)}^{u} \Sigma_{s}\left(u^{\prime}\right) \Phi\left(u^{\prime}\right) d u^{\prime}
\end{array}\right]
\end{aligned}
$$

Photo 5.5 Mireille Coste-
Delclaux is France's foremost specialist on selfshielding, a field in which the French CEA have always produced notable experts (Courtesy Coste)


Fig. 5.10 Example of group subdivision: group 5 is divided into 4 subgroups $W(2$ to 5.5$)$. Note that some neutrons in group 2 (with low lethargy) cannot reach group 5


The integrals can now be substituted by the average value of the scattering rate multiplied by the lethargy range:
or:

$$
\begin{aligned}
& R_{c}\left[\Phi^{T R}\right]=\frac{1}{\varepsilon_{c}}\left[\overline{\Sigma_{s} \Phi_{g^{\prime}}}\left(u_{\max }\left(g^{\prime}\right)-\left(u-\varepsilon_{c}\right)\right)+\sum_{g^{\prime \prime}=g^{\prime}+1}^{g^{\prime \prime}=g-1} \overline{\Sigma_{s} \Phi_{g^{\prime \prime}}}\left(u_{\max }\left(g^{\prime \prime}\right)-u_{\min }\left(g^{\prime \prime}\right)\right)\right. \\
& +{\left.\overline{\Sigma_{s}} \boldsymbol{\Phi}_{g}\left(u-u_{\min }(g)\right)\right]}
\end{aligned}
$$

The microscopic operator may be deduced directly by replacing the flux by the fine structure $\varphi$. Analysis of the last equation demonstrates that the weighting of the scattering rates, which is proportional to the difference in lethargy (divided by the maximum gain in lethargy), is in fact the mean probability of reaching group $g$ from $g^{\prime}$, i.e.:

$$
\begin{aligned}
r_{c}\left[\varphi^{T R}\right]= & \frac{1}{\varepsilon_{c}}\left[{\left.\overline{\Sigma_{s}} \varphi_{g^{\prime}}\left(u_{\max }\left(g^{\prime}\right)-\left(u-\varepsilon_{c}\right)\right)+\sum_{g^{\prime \prime}=g^{\prime}+1}^{g^{\prime \prime}=g-1}{\overline{\Sigma_{s}} \varphi_{g^{\prime \prime}}\left(u_{\max }\left(g^{\prime \prime}\right)-u_{\min }\left(g^{\prime \prime}\right)\right)}+{\overline{\Sigma_{s} \varphi}}_{g}\left(u-u_{\min }(g)\right)\right]=\sum_{g^{\prime} \leq g} p\left(g^{\prime} \rightarrow g\right){\overline{\Sigma_{s}} \varphi_{g^{\prime}}}} .\right.
\end{aligned}
$$

The $T R$ model converges towards the exact slowing-down operator of the heavy nuclide as the number of groups increases.


Fig. 5.11 Depression of flux as a function of resonances: the spatial flux in the fuel rod and that in the moderator are presented at different energies (arbitrary ordinates axis). The flux is depressed for energies corresponding to the resonances of uranium 238. At the fission energy, the fast flux is prevalent in the fuel. The thermal flux is more significant in the moderator than in the fuel. See also (Duderstadt and Hamilton 1976, p. 400)

### 5.7 Heterogeneous Medium

(Dresner 1960, p. 61)

### 5.7.1 Two-Media Problem

In the computation of industrial cores, the problems generally involve heterogeneous lattices. Can the same process be used as for homogeneous media?

Let us consider two media:

- A fuel medium of index $c$ (for combustible) with one resonant isotope $\left(\Sigma_{t}^{c}, N_{c}\right)$;
- An external moderator medium of index $M$ with one light isotope such that $\Sigma_{t}^{M} \approx \Sigma_{s}^{M}$ varies slowly.

Postulating flat flux in each medium and isotropic collisions in the center of mass, the neutron balance, written in a notation first proposed by J. Chernick (1955) ${ }^{17}$ (Fig. 5.11), is:

[^94]\[

\left\{$$
\begin{array}{cl}
V_{c} \Sigma_{t}^{c} \Phi_{c}=V_{c} P_{c c} R_{c}\left[\Phi_{c}\right]+V_{M} P_{M c} R_{M}\left[\Phi_{M}\right] & \text { for the resonant medium } \\
V_{M} \Sigma_{t}^{M} \Phi_{M}=V_{c} P_{c M} R_{c}\left[\Phi_{c}\right]+V_{M} P_{M M} R_{M}\left[\Phi_{M}\right] & \text { for the moderator }
\end{array}
$$\right.
\]

where:
$V_{i}$ the volume of medium $i$;
$\Phi_{i}$ the flux in this medium;
$P_{i j}$ the first-collision probability ${ }^{18}$ in medium $j$ for a neutron emitted in medium $i$.

$M$ external moderator
c resonant isotope medium
Let us consider the phenomena occurring in the fuel medium and use the same approximations as those applied to the homogeneous case:

$$
R_{M}\left[\Phi_{M}\right] \approx \Sigma_{M} \Psi \Phi_{c}=\Psi \varphi_{c} R_{c}\left[\Phi_{c}\right] \approx \Psi R_{c}\left[\varphi_{c}\right]
$$

with the hypothesis of a uniform spatial macroscopic flux. Using the reciprocity properties and conserving the collision probabilities (leakage of neutrons is assumed to be zero):

$$
\left\{\begin{array}{lc}
V_{M} P_{M c} \Sigma_{s}^{M}=V_{c} P_{c M} \Sigma_{t}^{c} & \text { reciprocity property } \\
P_{c M}=1-P_{c c} & \left(\sum_{j} P_{i j}=1\right)
\end{array}\right.
$$

The balance over the resonant isotope is written as:

$$
V_{c} \Sigma_{t}^{c} \Psi \varphi_{c}=V_{c} P_{c c} \Psi R_{c}\left[\varphi_{c}\right]+V_{M} P_{M c} \Sigma_{s}^{M} \Psi
$$

or: $V_{c} P_{c c} R_{c}\left[\varphi_{c}\right]+\underbrace{V_{M} P_{M c} \Sigma_{s}^{M}}_{V_{c} P_{c M} \Sigma_{t}^{c}}-V_{c} \Sigma_{t}^{c} \varphi_{c}=0$

[^95]Giving:

$$
\frac{1}{N_{c}} R_{c}\left[\varphi_{c}\right]-\frac{\sigma_{t}^{c}}{P_{c c}} \varphi_{c}+\frac{1-P_{c c}}{P_{c c}} \sigma_{t}^{c}=0
$$

Defining the equivalent cross section: $\sigma_{e} \equiv \sigma_{t}^{c} \frac{1-P_{c c}}{P_{c c}} \quad$ and the operator $r_{c}[] \equiv \frac{1}{N_{c}} R_{c}[]$
yields the fine structure equation for the homogeneous medium:
Heterogeneous fine structure equation: $r_{c}\left[\varphi_{c}\right]-\left(\sigma_{t}^{c}(u)+\sigma_{e}(u)\right) \varphi_{c}(u)+\sigma_{e}(u)=0$

Only the dilution $\sigma_{e}(u)$ is modified due to the heterogeneous effect. It depends on the resonant isotope and the moderator via the first collision probability $P_{00}$ in the fuel. The fine structure equation for lethargy was solved in a homogeneous medium using a homogeneous dilution cross section $\sigma_{e}=\Sigma_{s}^{M} / N_{c}$, which is constant where $\Sigma_{s}^{M}$ is practically constant. This is not true of the heterogeneous medium since $\sigma_{e}(u)$ depends on lethargy through the term $\sigma_{t}^{c}(u)$. To obtain a similar equation to the homogeneous case and utilize the same resolution process, the problem must be characterized by a parameter that does not depend on energy, $\bar{\sigma}_{e}$, the equivalent homogeneous cross section, or true equivalent cross section. The correct averaging method consists not in averaging $\sigma_{e}(u)$ over the lethargy range, but rather in conserving the effective resonance integral for the reaction in question.

The evolution of $\sigma_{e}$ as a function of $\sigma_{t}^{c}$ shows that the equivalent cross section does not vary significantly where the variation $\sigma_{t}^{c}$ varies by several decades. Hence, with little loss of precision in calculating the fine structure, the value of $\sigma_{e}(u)$ can be approximated on a lethargy interval by $\bar{\sigma}_{e}=a_{\text {Bell }} \sigma_{e, \infty}$, where the coefficient $a_{\text {Bell }}$ is the Bell factor ${ }^{19}$ (Reuss 2008, p. 243), and $\sigma_{e, \infty}=\lim _{\sigma_{0} \rightarrow+\infty} \sigma_{e}\left(\sigma_{0}\right)$ (Figs. 5.12 and 5.13; Photo 5.6).

Figure 5.14 gives $\bar{\sigma}_{e} / \sigma_{e, \infty}$ as a function of the product $R_{c y l} \Sigma_{t}^{c}$ ( $R_{c y l}$ being the radius of the fuel rod). A mean value of 1.16 for the Bell factor accurately represents the geometry of both rods and slabs (Stamm'ler and Abbate 1983, p. 297). Therefore, to be able to use in any situation the tabulated effective cross sections as a function of $\sigma_{e}$, which have been established in homogeneous cases, the homogenous equivalent of the heterogeneous case is required. To this end, $\bar{\sigma}_{e}$ is

[^96]

Fig. 5.12 Evolution of the Bell factor for a cylindrical fuel rod


Fig. 5.13 Heterogeneous/homogeneous equivalence


Photo 5.6 George Irving Bell (circa 1960, Public domain)
determined using an average constant which, in the homogeneous case, gives the same effective integral as that computed in heterogeneous geometry, namely:

$$
I_{e f f}^{\text {homogeneous } g}\left(\bar{\sigma}_{e}\right) \equiv I_{e f f}^{g}\left(\sigma_{e}(u)\right)
$$

For example, for an absorption reaction and using the $N R$ approximation:

$$
I_{a_{e f f}}^{N R}=\int_{u} \sigma_{a}(u) \varphi^{N R}(u) d u=\int_{u} \sigma_{a}(u) \frac{\sigma_{p}+\sigma_{e}(u)}{\sigma_{t}^{c}(u)+\sigma_{e}(u)} d u \equiv \int_{u} \sigma_{a}(u) \frac{\sigma_{p}+\bar{\sigma}_{e}}{\sigma_{t}^{c}(u)+\bar{\sigma}_{e}} d u
$$

Once the equivalent cross section is obtained, the problem is reduced to a homogeneous case and through interpolations in the homogeneous tables from a refined energy mesh (Fig. 5.13):

In the initial versions of the French APOLLO1 code, which incorporated the Livolant-Jeanpierre model, several approximations have been set up:

- Equivalence is performed globally (rather than group by group) for the complete domain $G$ in which the large resonances of the nuclide are found. The effective absorption integral is conserved:

$$
I_{a, e f f}^{\text {homogeneous }}{ }^{G}\left(\bar{\sigma}_{e}\right)=I_{a, \text { eff }}^{G}\left(\sigma_{e}\right)
$$

- Calculation of the effective integrals is performed using the $N R$ approximation for the slowing-down component.

Using the fine structure term in the $N R$ hypothesis:

$$
\left\{\begin{array}{l}
r_{c}\left[\varphi_{c}\right]-\left(\sigma_{t}^{c}(u)+\sigma_{e}(u)\right) \quad \varphi_{c}(u)+\sigma_{e}=0 \\
r_{c} \varphi_{c} \approx \sigma_{p} \quad \varphi_{\text {asymp }} \approx 1 \\
\varphi_{c} \approx \frac{\sigma_{p}+\sigma_{e}(u)}{\sigma_{t}^{c}(u)+\sigma_{e}(u)} \int_{G} \sigma_{a}(u) \frac{\sigma_{p}+\bar{\sigma}_{e}}{\sigma_{t}^{c}(u)+\bar{\sigma}_{e}} d u=\int_{G} \sigma_{a}(u) \frac{\sigma_{p}+\sigma_{e}(u)}{\sigma_{t}^{c}(u)+\sigma_{e}(u)} d u
\end{array}\right.
$$

### 5.7.2 Accounting for Spatial Interaction

If the resonant isotope is distributed homogeneously in the same medium, the equivalent cross section $\sigma_{e}$ is a function of $P_{c c}$, i.e. the probability that a neutron emitted in a medium containing the resonant isotope will undergo its first collision with a nuclide of the same type. Where the resonant isotope is found in several geometrical zones in which concentrations are not the same, the probability $P_{c c}$ cannot fully characterize what actually takes place in the fuel.

Indeed, from Fig. 5.14, it may be deduced that the probability of a neutron undergoing its first collision with the resonant nuclide in any of the fuel regions (1,2 or 3) will differ according to whether it is emitted in 3 or 1 (at the center of 1 , its chances of escaping the resonances of the isotope are obviously lower). To allow for this phenomenon, the self-shielding of the heavy nuclide is calculated using the PIC formalism. Let $N$ be the number of resonant fuel regions (containing only the resonant isotope) and $L$ (stands for Light nuclides) the number of pure moderator regions (with only moderating nuclides $(M)$ ). For each "resonant" region, $i=1, N$ :


Total cross section of the resonant
$\sum_{t}^{c j} \quad$ isotope in the $j$-th cross section of the resonant isotope.

Fig. 5.14 Zoning of fuel

$$
V_{i} \Sigma_{t}^{c, i} \quad \Phi_{c, i}=\sum_{j=1}^{N} \underbrace{V_{j} P_{j i} R_{c j}\left[\Phi_{c, j}\right]}_{\text {fuel regions }}+\sum_{k=1}^{L} \underbrace{V_{k} P_{k i} R_{M k}\left[\Phi_{M, k}\right]}_{\text {moderator regions }}
$$

where:
$\Sigma_{t}^{c, i}$ is the total cross section of the resonant isotope in region $i$ (not to be confused with the total cross section of medium $i$, since it is the sole nuclide in this region);
$\Sigma_{t}^{M, k}$ is the total cross section of the moderator in region $k$.

The corresponding fine structure equation with the same hypotheses discussed in the two-media heterogeneous medium is written as:

$$
V_{i} \Sigma_{t}^{c, i} \varphi_{c, i}=\sum_{j=1}^{N} V_{j} P_{j i} R_{c}\left[\varphi_{c, j}\right]+\sum_{k=1}^{L} V_{k} P_{k i} \Sigma_{t}^{M, k} \quad \text { for each cell } i
$$

The slowing-down operator in the fuel is the same in all fuel regions since there is only one resonant isotope. First, using the reciprocity principle between region $i$ and the other resonant regions $j$;

$$
P_{j i} V_{j} \Sigma_{t}^{c, j}=P_{i j} V_{i} \Sigma_{t}^{c, i}
$$

Further, between region $i$ and the moderator regions:

$$
P_{k i} V_{k} \Sigma_{t}^{M, k}=P_{i k} V_{i} \Sigma_{t}^{c, i}
$$

The $N$ equations system gives:

$$
\begin{equation*}
\Sigma_{t}^{c, i} \quad \varphi_{c, i}=\sum_{j=1}^{N} P_{i j} \frac{\Sigma_{t}^{c, i}}{\Sigma_{t}^{c, j}} R_{c}\left[\varphi_{c, j}\right]+\Sigma_{t}^{c, i} \sum_{k=1}^{L} P_{i k} \quad \text { where } i=1, N \tag{5.10}
\end{equation*}
$$

The PIC method hinges on the hypothesis that the slowing-down operator is proportional to the resonant nuclide cross section:

$$
\begin{equation*}
\text { PIC hypothesis : } \quad \frac{R_{c}\left[\varphi_{c, i}\right]}{\Sigma_{t}^{c, i}} \approx \frac{R_{c}\left[\phi_{c, j}\right]}{\Sigma_{t}^{c, j}} \tag{5.11}
\end{equation*}
$$

This hypothesis is exact in the $N R$ approximation. The normalization closure for the first collision probabilities without leakage is written as:

$$
\sum_{j=1}^{N} P_{i j}+\sum_{k=1}^{L} P_{i k}=1
$$

Under these assumptions, Eq. (5.10) is simplified by using the PIC hypothesis and factorizing by the constant term:

$$
\varphi_{c, i}=\frac{R_{c}\left[\varphi_{c, i}\right]}{\Sigma_{t}^{c, i}} \sum_{j=1}^{N} P_{i j}+\left(1-\sum_{j=1}^{N} P_{i j}\right)
$$

The new probability of leakage inside the fuel is:

$$
P_{i c}=\sum_{j=1}^{N} P_{i j}
$$

Hence the term PIC method. It accounts for a neutron emitted in region $i$ and undergoing a collision with the resonant isotope in the fuel regions $j$. Thus:

$$
R_{c}\left[\varphi_{c, i}\right]-\frac{\Sigma_{t}^{c, i}}{P_{i c}} \varphi_{0 i}+\frac{1-P_{i c}}{P_{i c}} \quad \Sigma_{t}^{c, i}=0,
$$

which, when divided by $N_{c, i}$ leads to:
Fine structure equation in zone $i: \frac{R_{c}}{N_{c, i}}\left[\varphi_{c, i}\right]-\left(\sigma_{e, i}+\sigma_{t, i}^{c}\right) \quad \varphi_{c, i}+\sigma_{e, i}=0$
with: $\quad \sigma_{e, i}=\sigma_{t, i}^{c} \frac{1-P_{i c}}{P_{i c}} \quad, \sigma_{t, i}^{c}=\frac{\Sigma_{t, i}^{c}}{N_{c, i}}$
and $N_{c, i}$ is the concentration of the resonant isotope in the medium $i$. For each region $i$, the solution to the equation $I_{a}^{\text {heterogeneoous, } G} \quad\left(\overline{\sigma_{e, i}}\right)=I_{a}^{G} \quad{ }_{e f f}\left(\sigma_{e, i}\right)$ leads to the
true equivalent cross section $\overline{\sigma_{e, i}}$ in a scheme similar to that of the two-region heterogeneous model. Thus:

$$
\sigma_{e, i}^{G} \quad \rightarrow \overline{\sigma_{e, i}} \rightarrow \sigma_{e f f, \quad i}^{g}
$$

The heterogeneous problem for $N+L$ regions is thus transformed into $N$ heterogeneous two-region problems, one the fuel and the other the moderator. This method allows the calculation of $N$ fine structures, where, if one is known, the others may be deduced using the PIC model.

### 5.7.3 Generalization to Several Self-Shielding Regions

For a heterogeneous geometry where the $N$ media all comprise the same resonant isotope, $U$, and the moderator nuclide $m$ (there may be several moderators, but only one term is employed), the balance is written as:

$$
V_{i} \Sigma_{t}^{i} \Phi_{i}=\sum_{j=1}^{N} V_{j} P_{j i} \quad\left(R_{c j}\left[\Phi_{j}\right]+R_{m j}\left[\Phi_{j}\right]\right)
$$

As with the infinite homogeneous medium, the flux is developed as macroscopic flux $\Psi$ and microscopic $\varphi$ flux, although these quantities are now space-dependent: $\Phi_{i}=\Psi_{i} \varphi_{i}$. The resonant isotope slowing-down operator (which is short-range) is written as:

$$
R_{c j}\left[\Phi_{j}\right] \approx \Psi_{i} R_{c j}\left[\varphi_{j}\right]
$$

As with the homogeneous case, we may also write: $R_{m j}\left[\Phi_{j}\right]=\Sigma_{m, j} \Psi_{j}$, where $\Sigma_{m, j}$ is the scattering cross section for all moderator isotopes $m$ in region $j$. The problem may be simplified using an important supplementary hypothesis: the macroscopic flux does not depend on space. This hypothesis, which appears strong, has in fact been experimentally confirmed. The equation then simplifies to:

$$
V_{i} \Sigma_{t}^{i} \varphi_{i}=\sum_{j=1}^{N} V_{j} P_{j i} \quad\left(R_{c j}\left[\varphi_{j}\right]+\Sigma_{m, j}\right)
$$

A self-shielded region, denoted $\alpha$, is conventionally defined by grouping the computation regions containing the resonant isotope $U$ at a given temperature. The summation over all the media $i$ belonging to region $\alpha$ gives:

$$
\begin{aligned}
\sum_{i \in \alpha} V_{i} \Sigma_{t}^{i} \varphi_{i}= & \sum_{i \in \alpha} \sum_{j=1}^{N} V_{j} P_{j i}\left(R_{c j}\left[\varphi_{j}\right]+\Sigma_{m, j}\right) \\
= & \sum_{i \in \alpha} \sum_{\beta=1}^{B} \sum_{j \in \beta} V_{j} P_{j i}\left(R_{c j}\left[\varphi_{j}\right]+\Sigma_{m, j}\right) \\
& +\sum_{i \in \alpha} \sum_{j \notin \beta, \forall \beta} V_{j} P_{j i}(\underbrace{R_{c j}\left[\varphi_{j}\right]}_{0}+\Sigma_{m, j})
\end{aligned}
$$

The geometry is decomposed into $B$ self-shielding options. These regions do not necessarily cover the entire geometry, leaving $L$ media that are purely moderating, and which may be defined as $j \notin \beta, \forall \beta$. In these media without resonant isotopes, the fine structure is zero, hence $\forall j \notin \beta, \forall \beta, R_{c j}\left[\varphi_{j}\right]=0$. By definition, all the constituent isotopes of a self-shielded region have the same microscopic cross sections, and thus the same microscopic slowing-down operator, $r_{c j}\left[\varphi_{j}\right]$. The last step consists in assigning each medium to a self-shielded region having the same flux, $\varphi_{\alpha}$, which is the average flux of the concordant mean flux over all considered media. The fine structure equation, which is in fact a linear system, is written as:

Heterogeneous fine structure equations:

$$
\begin{equation*}
\left(\sum_{i \in \alpha} V_{i} \Sigma_{t}^{i}\right) \varphi_{\alpha}=\sum_{i \in \alpha} \sum_{\beta=1}^{B} \sum_{j \in \beta} V_{j} P_{j i} N_{U, j} r_{\beta}\left[\varphi_{\beta}\right]+\sum_{i \in \alpha} \sum_{j} V_{j} P_{j i} \Sigma_{m, j} \tag{5.13}
\end{equation*}
$$

The PIC formalism, seen above, artificially leads to a diagonal term, which is the heavy slowing-down term, although recent studies by Mireille Coste (1997) allow Eq. (5.13) to be solved using the Direct method. Leaving aside the details, this method consists in choosing one of the resonant isotope models seen earlier ( $N R$, $W R, S T$ or $T F$ ) and solving the linear system for all Eq. (5.13) for each self-shielded zone (in the case of the $N R$ and $W R$ models, a matrix must be inverted for each fuel zone ${ }^{20}$ ).

[^97]
### 5.8 Accounting for Energy Interactions: Self-Shielding of Mixtures

In the last examples, for simplicity, we considered a medium with only one fuel (usual index $c$ ), and one resonant nuclide. Absorption from the heavy nuclide is modified by the presence in fuel $c$ of the other isotopes with resonances. There is thus overlapping of resonances, which in practice means that a neutron absorbed by the resonant medium cannot be absorbed by another heavy nuclide. Assuming that the fuel is now constituted of nuclides $\alpha$ and $\beta$ (only two isotopes are considered, but generalization to any number of isotopes is possible), the neutron balance equations are written with the slowing down for both resonant isotopes:
$\left\{\begin{array}{l}V_{c} \Sigma_{t}^{c} \Phi_{c}=V_{c} P_{c c}\left(R_{\alpha}\left[\Phi_{c}\right]+R_{\beta}\left[\Phi_{c}\right]\right)+V_{M} P_{M c} R_{M}\left[\Phi_{M}\right] \quad \text { for the fuel medium } \\ V_{M} \Sigma_{t}^{M} \Phi_{M}=V_{c} P_{c M}\left(R_{\alpha}\left[\Phi_{c}\right]+R_{\beta}\left[\Phi_{c}\right]\right)+V_{M} P_{M M} R_{M}\left[\Phi_{M}\right] \quad \text { for the moderator }\end{array}\right.$
As for the previous approaches, the effects for the fuel and the moderator are written as:

$$
\left\{\begin{array}{cc}
R_{M}\left[\Phi_{M}\right]=\Sigma_{s}^{M} \psi & \Phi_{c}=\varphi_{c} \psi \\
R_{\alpha}\left[\Phi_{c}\right]=\psi R_{\alpha}\left[\Phi_{c}\right] & R_{\beta}\left[\Phi_{c}\right]=\psi R_{\beta}\left[\Phi_{c}\right]
\end{array}\right.
$$

The simplest way of considering the problem is that each resonant isotope is treated separately from the other nuclides, with the latter being taken as non-absorbing moderators (which is not a valid hypothesis if the heavy nuclides are highly absorbing) and with slowly-varying total cross sections (i.e. $R_{\beta}\left[\varphi_{c}\right] \approx \Sigma_{\beta}$ ), which are added to the initial moderator. The problem is thus transformed into the earlier case, and using the reciprocity principle ( $V_{M} P_{M c} \Sigma_{s}^{M}$ $\left.=V_{c} P_{c M}\left(\Sigma_{t}^{\alpha}(u)+\Sigma_{t}^{\beta}\right)\right)$ for the collision probabilities, the following equations are obtained using $V_{M} P_{M c} \Sigma_{s}^{M}=V_{c} P_{c M}\left(\Sigma_{t}^{\alpha}(u)+\Sigma_{t}^{\beta}\right)$ :

$$
R_{\alpha}\left[\varphi_{c}\right]-\frac{\left(\Sigma_{t}^{\alpha}(u)+\Sigma_{t}^{\beta}\right)}{P c c} \varphi_{c}(u)+\Sigma_{t}^{\beta}+\frac{1-P_{c c}}{P_{c c}}\left(\Sigma_{t}^{\alpha}(u)+\Sigma_{t}^{\beta}\right)=0
$$

by setting the equivalent cross section for two regions as $\Sigma_{e}(u) \equiv$ $\left(1-P_{c c}\right)\left(\Sigma_{t}^{\alpha}(u)+\Sigma_{t}^{\beta}\right) / P_{c c}$. If a new equivalent cross section for the mixture of nuclides $\alpha+\beta$ is defined as:

$$
\widetilde{\Sigma}_{e}(u) \equiv \Sigma_{t}^{\beta}+\frac{1-P_{c c}}{P_{c c}}\left(\Sigma_{t}^{\alpha}(u)+\Sigma_{t}^{\beta}\right)
$$

The exact heterogeneous equation for two regions is obtained:

$$
R_{\alpha}\left[\varphi_{c}\right]-\left(\Sigma_{t}^{\alpha}(u)+\widetilde{\Sigma}_{e}(u)\right) \varphi_{c}(u)+\widetilde{\Sigma}_{e}(u)=0
$$

This result calls for several remarks. First, the extension to several heavy nuclides is obtained directly as:

$$
\Sigma_{t}^{c}=\Sigma_{t}^{\alpha}+\sum_{x} \Sigma_{x}
$$

substituting $\Sigma_{t}^{\beta}$ by $\sum_{x} \Sigma_{x}$ in the previous formulae. Further, the fine flux resulting from the computation of self-shielded cross sections of a nuclide $\alpha$ can be used to compute the self-shielded cross sections of another nuclide $\beta$. However, the result will differ depending on the order in which the nuclides are self-shielded. The latter remark is unsatisfactory from a scientific perspective. The mutual interaction of nuclides is accounted for in the computation of $\sigma_{e}$ with the use of self-shielded cross sections of nuclides already being considered for $\Sigma_{x}$. Thus, the order of selfshielding is important and the process should start with the most important isotopes such as $\Sigma_{a}\left({ }_{92}^{238} U\right)$, followed by $\Sigma_{a}\left({ }_{92}^{235} U\right)$ and $\Sigma_{a}\left({ }_{94}^{239} \mathrm{Pu}\right)$ so as to reduce the impact of the methodology. An iterative procedure in collision probabilities is used to carry out the self-shielding process. However, this can be quite onerous since the iterative process depends on the cross sections, which must be recomputed at each iteration. The iteration continues up to convergence of the self-shielded cross sections. Temperature effects will be discussed at the end of the chapter when discussing the resonant absorption integral after the Doppler effect has been introduced.

### 5.9 Intermediate Resonance Model in Flux Calculations

(Stamm'ler and Abbate 1983, p. 305)
In all of the foregoing models, the $N R$ hypothesis was widely employed to represent not just the slowing-down operator for the moderator, which is warranted, but in some cases for the fuel also. Unfortunately, this hypothesis cannot be used in all cases. In this section, the Intermediate Resonance (IR) model will be considered for slowing-down operators. Let us consider that the fuel consists of resonant heavy nuclides $U$ with moderator $m$, surrounded by an external moderator $M$ (Fig. 5.15):

Starting from the neutron balance in the fuel and the moderator:

Here we shall use the Wigner rational approximation (Weinberg and Wigner 1958; Dresner 1960, p. 60) for the escape probability from the rod as a function of the leakage cross section $\bar{\Sigma}_{e}$ (not to be confused with the equivalent cross section,


Fig. 5.15 Geometry of two regions and three media
hence the symbol $\leftrightarrow$ ), while conserving all generality. For a clear understanding, the probability is expressed in terms of energy rather than in lethargy:

$$
\begin{equation*}
\text { Wigner rational approximation : } \quad P_{c M}=\frac{\stackrel{\Sigma}{\Sigma}_{e}}{\Sigma_{t}^{c}(E)+\stackrel{\rightharpoonup}{\Sigma}_{e}} \tag{5.14}
\end{equation*}
$$

In this formula, $\stackrel{\rightharpoonup}{\Sigma}_{e}$ represents the fact that a neutron can leak from the geometry and that the escape probability can still be written as the ratio of leakage to total absorption and leakage (Stamm'ler et Abbate 1983, p. 299). The reciprocity principle of probabilities leads to:

$$
P_{c M} V_{c} \Sigma_{t}^{c}(E)=P_{c M} V_{c}\left(\Sigma_{t}^{U}(E)+\Sigma_{s}^{m}\right)=P_{M c} \quad V_{M} \Sigma_{t}^{M} \approx P_{M c} V_{M} \Sigma_{s}^{M}
$$

These two relations are inserted in the balance after simplifying the slowingdown operators in similar fashion:

$$
\begin{gathered}
R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right]= \begin{cases}\frac{\Sigma_{s}^{M}}{E} & \text { NR hypothesis } \\
\Sigma_{s}^{M} \Phi_{M}(E) & \text { WR hypothesis }\end{cases} \\
R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]=R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+R_{m}\left[\Sigma_{s}^{m} \Phi_{c}\right]=R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+\Sigma_{s}^{m} R_{m}\left[\Phi_{c}\right]
\end{gathered}
$$

and using the following equations obtained after some mathematical simplifications:

$$
\left\{\begin{array}{l}
\Sigma_{t}(E)=\frac{\Sigma_{e}\left(1-P_{c M}(E)\right)}{P_{c M}(E)}=\left(\Sigma_{t}(E)+\stackrel{\rightharpoonup}{\Sigma}_{e}\right)\left(1-P_{c M}(E)\right) \\
1-P_{c M}(E)=\frac{\Sigma_{t}(E)}{\Sigma_{t}(E)+\stackrel{\rightharpoonup}{\Sigma}_{e}} \\
1-P_{M c}(E)=1-\frac{V_{c} \Sigma_{t}^{c} \Sigma_{e}}{V_{M} \Sigma_{s}^{M}\left(\Sigma_{t}(E)+\stackrel{\Sigma}{\Sigma}_{e}\right)}
\end{array}\right.
$$

The following equations are obtained:

$$
\left\{\begin{array}{l}
\left(\Sigma_{t}(E)+\vec{\Sigma}_{e}\right) \Phi_{c}=R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+\Sigma_{s}^{m} R_{m}\left[\Phi_{c}\right]+\vec{\Sigma}_{e} R_{M}\left[\Phi_{M}\right] \\
\left(\Sigma_{t}(E)+\vec{\Sigma}_{e}\right) \Phi_{M}=\frac{V_{c} \Sigma_{e}}{V_{M} \Sigma_{s}^{M}}\left(R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+\Sigma_{s}^{m} R_{m}\left[\Phi_{c}\right]\right) \\
+\left(\left(\Sigma_{t}(E)+\vec{\Sigma}_{e}\right)-\frac{V_{c} \Sigma_{t}(E) \Sigma_{e}}{V_{M} \Sigma_{s}^{M}}\right) R_{M}\left[\Phi_{M}\right]
\end{array}\right.
$$

The $I R$ hypothesis consists in expressing the moderator slowing-down operator in the form of a "linear interpolation" between wide and narrow resonances:

$$
R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right]=\lambda \frac{\sum_{s}^{M}}{E}+(1-\lambda) \Sigma_{s}^{M} \Phi_{M}(E)
$$

Thus, the flux can be computed analytically in the moderator $M$ as a function of the flux in the fuel:

$$
\Phi_{M}(E)=K\left(\Phi_{c}(E)+\lambda \frac{1-\beta}{\beta E}\right) \quad \text { with }: \quad\left\{\begin{array}{l}
K=\frac{\beta}{\lambda+(1-\lambda) \beta} \\
\beta=\frac{V_{c} \Sigma_{e}}{V_{M} \Sigma_{s}^{M}}
\end{array}\right.
$$

Substituting the $M$ moderator flux in the first neutron balance, the integral equation for $\Phi_{c}(E)$ is obtained:

$$
\begin{aligned}
\left(\Sigma_{t}(E)+\stackrel{\Sigma}{\Sigma}_{e}\right) \Phi_{c}(E)= & R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+\Sigma_{s}^{m} R_{m}\left[\Phi_{c}\right] \\
& +\Sigma_{e}\left(\lambda \frac{\Sigma_{s}^{M}}{E}+(1-\lambda) \Sigma_{s}^{M} K\left(\Phi_{c}(E)+\lambda \frac{1-\beta}{\beta E}\right)\right)
\end{aligned}
$$

which can be shortened to:
Flux equation for fuel in the $I R$ approximation : $\quad\left(\Sigma_{t}(E)+\widetilde{\Sigma}_{e}\right) \Phi_{c}(E)$

$$
\begin{equation*}
=R_{U}\left[\Sigma_{s}^{U}(E) \Phi_{c}(E)\right]+\Sigma_{s}^{m} R_{m}\left[\Phi_{c}(E)\right]+\lambda\left(\frac{1-\beta}{\beta}\right) K \frac{\widetilde{\Sigma}_{e}}{E} \tag{5.15}
\end{equation*}
$$

where: $\widetilde{\Sigma}_{e}=\overleftrightarrow{\Sigma}_{e}(1-(1-\lambda) K)$. Similarly, a flux equation could be written for $M$ showing the uncoupling of the two fluxes via the $I R$ hypothesis and the rational approximation. Evaluation of the parameter $\lambda$ will be discussed in the chapter on the Doppler effect.

### 5.10 The Probability Table Method

In 1970, a Russian team (Nicolaevand Khokhlov) proposed ${ }^{21}$ a method to take account of resonances called the subgroup method, but popularly referred to as probability tables. ${ }^{22,23}$ This method was developed in France by Pierre Ribon (CEA/Saclay), ${ }^{24}$ A. Khairallah and J. Recolin (CEA/Cadarache). Ribon significantly improved the precision of the method through the use of optimal quadrature. It consisted in discretizing cross sections using discretely-occurring line density

[^98]
(Courtesy Ribon)
distributions rather than the more natural energy variable. To illustrate this discretization, let us consider a cross section (Fig. 5.16). For a given value of the cross section between $\sigma_{\min }$ and $\sigma_{\max }$, the occurrence rate, $\pi(\sigma)$, also known as the distribution function, is computed and normalized either to the energy range, $E_{\max }-E_{\min }$, or to the lethargy range.

Using this approach, the occurrence rate for the minimum value of the cross section is $\pi\left(\sigma_{\min }\right)=1$. The probability density $p(\sigma) d \sigma$ is defined as the derivative of the distribution function. The distribution ${ }^{25}$ obtained is then discretized using discrete lines ( 3 in this example). Instead of the position of the resonances, a table of discrete values for the cross sections $\sigma_{i}$ with the weights $\pi_{i}$ is employed (Fig. 5.17).


Fig. 5.16 Construction of the distribution function


Fig. 5.17 Probability table $p(\sigma)$ (from Alain Hébert and Mireille Coste, Courtesy Coste)

[^99]These weights can be normalized to obtain a probability density $p(\sigma)$ such that:

$$
\begin{gathered}
\int_{0}^{\max (\sigma)} p(\sigma) d \sigma=1 \\
\pi(\sigma)=\frac{\sum_{i}\left(E_{i+1}-E_{i}\right)}{E_{\max }-E_{\min }} \quad \text { for }\left\{\begin{array}{l}
\sigma_{t}\left(E_{i+1}\right)=\sigma \\
\sigma_{t}\left(E_{i}\right)=\sigma \\
\forall E \in\left[E_{i}, E_{i+1}\right]
\end{array} \quad \sigma_{t}(E)>\sigma\right.
\end{gathered}
$$

This change in variable enables the calculation of any integral of a function of variable $\sigma$ by a discrete sum over the discrete rays using the Lebesgue method [see (Diu et al. 2001, p. 55)] for change in variables for probability densities):

$$
I=\int_{u_{\min }}^{u_{\max }} f(\sigma(u)) d u=\int_{\sigma_{\min }}^{\sigma_{\max }} f(\sigma) p(\sigma) d \sigma \approx \sum_{i} f\left(\sigma_{i}\right) p_{i}
$$

and again, using the normalized probability density:

$$
\frac{1}{u_{\max }-u_{\min }} \int_{u_{\min }}^{u_{\max }} f(\sigma(u)) d u=\int_{0}^{\sigma_{\max }} f(\sigma) p(\sigma) d \sigma
$$

The integral can also be computed in the form of a quadrature. In 1990, Ribon proposed the use of a Gaussian quadrature, which conserves the moments of the total cross section (the quadrature is exact at order $n$ for any polynomial of degree lower or equal to $2 n-1$ ). The moment $k$ of the total cross section is given by:

$$
\int_{u_{\min }}^{u_{\max }} \sigma^{k}(u) d u=\sum_{i=1}^{n} \sigma_{i}^{k} p_{i}
$$

The LHS of this expression is the exact moment computed with the exact form of the cross section obtained from nuclear libraries with a refined energy grid, while the RHS is its representation with a quadrature. Instead of varying $k$ from 0 to $2 n-1$, Ribon prefers to use $k$ from $-n+1$ to $n$, resulting in better modeling of negative moments. Writing the previous equations for $-n+1 \leq k \leq n$ produces a system of $2 n-1$ equations that are linear in $p_{i}$ but non-linear in $\sigma_{i}$. This system enables calculation of the optimal couples for the required integrals. These are always positive and may be made temperature-dependent to take into account the Doppler effect, but it must be borne in mind that the integrals are not linear with respect to $\sigma_{i}$ for high order moments (mathematically, interpolations over
temperature cannot be carried out for $\sigma_{i}$ ). Use of the quadrature formulae greatly simplifies the integral calculations. However, partial cross sections (e.g. $\sigma_{(n, \gamma)}$ ) are slightly more complicated. In neutronics, they are always in linear forms such as:

$$
I_{x}=\int_{u_{\min }}^{u_{\max }} f\left(\sigma_{t}(u)\right) \quad \sigma_{x}(u) d u \quad \text { with, e.g., } \quad f\left(\sigma_{t}(u)\right)=\Phi(u)
$$

In this case, the following can be written:

$$
I_{x}=\int_{\sigma_{t, \text { min }}}^{\sigma_{t, \text { max }}} f\left(\sigma_{t}\right) d \sigma_{t} \int_{\sigma_{x, \text { min }}}^{\sigma_{x, \text { max }}} \omega\left(\sigma_{t}, \sigma_{x}\right) \sigma_{x} d \sigma_{x}=\int_{\sigma_{t, \text { min }}}^{\sigma_{t, \text { max }}} f\left(\sigma_{t}\right) p\left(\sigma_{t}\right) \sigma_{x}\left(\sigma_{t}\right) d \sigma_{t}
$$

where $\sigma_{x}\left(\sigma_{t}\right)=\int_{\sigma_{x, \text { min }}}^{\sigma_{x, \text { max }}} \frac{\omega\left(\sigma_{t}, \sigma_{x}\right)}{p\left(\sigma_{t}\right)} \sigma_{x} d \sigma_{x}$ and $q\left(\sigma_{x} \mid \sigma_{t}\right) \equiv \omega\left(\sigma_{t}, \sigma_{x}\right) / p\left(\sigma_{t}\right)$ is the conditional probability of obtaining $\sigma_{x}$ where $\sigma_{t}$ is known. With quadratures, the integral value is:

$$
I_{x}=\sum_{i} p_{i} f\left(\sigma_{t, i}\right) \sigma_{x, i}
$$

The couples $\left(\sigma_{x, i}, p_{i}\right)$ are obtained by equating the first $n$ moments:

$$
\sum_{i} p_{i} \sigma_{t, i}^{k} \sigma_{x, i}=\int \sigma_{t}^{k}(u) \sigma_{x}(u) d u
$$

As seen earlier, it is more reasonable to vary $k$ from $-n / 2$ to $+n / 2$. Such a method for partial cross sections verifies that for each line $\sigma_{t, i}=\sum_{x} \sigma_{x, i}$. Hence, the probability table formalism can be applied to multi-group cross sections:

$$
\sigma_{x, g} \equiv \frac{\int_{\Delta u_{g}} \sigma_{x}(u) \Phi(u) d u}{\int_{\Delta u_{g}} \Phi(u) d u}
$$

with $\Phi(u)=R(u) /\left(\sigma_{t}(u)+\sigma_{e}\right)$ where $R(u)$ is the collision density. The integral at the numerator is computed using the method encountered earlier:

$$
\begin{aligned}
I_{x} & =\int_{\Delta u_{g}} \sigma_{x}(u) \Phi(u) d u \\
& =\int_{\Delta u_{g}} \sigma_{x}(u) \frac{1}{\sigma_{t}(u)+\sigma_{e}} R(u) d u=\int_{\Delta \sigma_{t}} \frac{1}{\sigma_{t}+\sigma_{e}} d \sigma_{t} \int_{\Delta \sigma_{x}} \sigma_{x} d \sigma_{x} \int_{\Delta R} R \omega\left(\sigma_{t}, \sigma_{x}, R\right) d R
\end{aligned}
$$

With $\omega\left(\sigma_{t}, \sigma_{x}, R\right) \equiv p\left(\sigma_{t}\right) q\left(\sigma_{x} \mid \sigma_{t}\right) r\left(R\left|\sigma_{x}\right| \sigma_{t}\right), r\left(R\left|\sigma_{x}\right| \sigma_{t}\right)$ being the probability of obtaining R where $\sigma_{x}$ and $\sigma_{t}$ are known. Therefore:

$$
I_{x}=\int_{\Delta \sigma_{t}} \frac{1}{\sigma_{t}+\sigma_{e}} p\left(\sigma_{t}\right) d \sigma_{t} \int_{\Delta \sigma_{x}} \sigma_{x} q\left(\sigma_{x} \mid \sigma_{t}\right) d \sigma_{x} \int_{\Delta R} \operatorname{Rr}\left(R\left|\sigma_{x}\right| \sigma_{t}\right) d R
$$

This expression can be simplified if we assume $r\left(R\left|\sigma_{x}\right| \sigma_{t}\right)$ to be independent of $\sigma_{x}$ and $\sigma_{t}$; this is the statistical hypothesis. In simple terms, the statistical hypothesis implies that the result is not influenced by the permutation of resonances in the energy range being considered. ${ }^{26}$ In this case, the last integral is simply the mean value of the collision density:

$$
\int_{\Delta R} R r\left(R\left|\sigma_{x}\right| \sigma_{t}\right) d R=\int_{\Delta R} R r(R) d R=\bar{R}
$$

Thus: $I_{x}=\bar{R} \int_{\Delta \sigma_{t}} \frac{1}{\sigma_{t}+\sigma_{e}} p\left(\sigma_{t}\right) \overline{\sigma_{x}} d \sigma_{t}=\bar{R} \sum_{i=1}^{n} \frac{1}{\sigma_{t, i}+\sigma_{e}} p_{i} \bar{\sigma}_{x, i}$
Let the cross section in the group be:

$$
\sigma_{x, g} \equiv \frac{\sum_{i=1}^{n} \frac{1}{\sigma_{t, i}+\sigma_{e}} p_{i} \bar{\sigma}_{x, i}}{\sum_{i=1}^{n} \frac{1}{\sigma_{t, i}+\sigma_{e}} p_{i}}
$$

The non-statistical hypothesis supposes that $r\left(R\left|\sigma_{x}\right| \sigma_{t}\right)$ does not depend solely on $\sigma_{t}$. The integral is written as:

$$
\begin{aligned}
I_{x} & =\int_{\Delta \sigma_{t}} \frac{1}{\sigma_{t}+\sigma_{e}} p\left(\sigma_{t}\right) d \sigma_{t} \int_{\Delta \sigma_{x}} \sigma_{x} q\left(\sigma_{x} \mid \sigma_{t}\right) d \sigma_{x} \int_{\Delta R} \operatorname{Rr}\left(R \mid \sigma_{x}\right) d R \\
& =\int_{\Delta \sigma_{t}} \frac{1}{\sigma_{t}+\sigma_{e}} p\left(\sigma_{t}\right) \overline{\sigma_{x}}\left(\sigma_{t}\right) \bar{R}\left(\sigma_{t}\right) d \sigma_{t}=\sum_{i=1}^{n} \frac{1}{\sigma_{t, i}+\sigma_{e}} p_{i} \bar{\sigma}_{x, i} \overline{R_{i}}
\end{aligned}
$$

with $\bar{\sigma}_{x, i}=\bar{\sigma}_{x}\left(\sigma_{t, i}\right)$ and $\overline{R_{i}}=\bar{R}\left(\sigma_{t, i}\right)$. Finally:

[^100]$$
\sigma_{x, g} \equiv \frac{\sum_{i=1}^{n} \frac{\overline{R_{i}}}{\sigma_{t, i}+\sigma_{e}} p_{i} \bar{\sigma}_{x, i}}{\sum_{i=1}^{n} \frac{\overline{R_{i}}}{\sigma_{t, i}+\sigma_{e}} p_{i}}
$$

The statistical hypothesis is obtained if all $\overline{R_{i}}$ are supposed to be equal to one another. The probability table method allows the conservation of data from the fine structure of cross sections and their fine condensation spectrum related to their condensation into groups. The Ribon moments method allows the same calculation with fewer energy groups than the initial subgroup method. It produces greater precision for effective reaction rates of important isotopes such as ${ }_{92}^{238} U$ and the selfshielding of complex cells. ${ }^{27}$

In conclusion, it should be kept in mind that the French school of neutronics is rich on the subject of self-shielding. Following the important founding concepts of Livolant and Jeanpierre, several novel works (Reuss, Tellier, Santamarina, Ribon, Coste) have brought the French spectral code into the international limelight. Reference studies ${ }^{28}$ have shown the discrepancies concerning the radiative capture rate of ${ }_{92}^{238} U$ between APOLLO2 and a hyperfine quasi-exact slowing-down calculation (TRAMP code, 32,256 energy groups between 7466 and 4 eV ) to be less than $1 \%$, leading to reactivity discrepancies of 100 pcm for a PWR cell. It should be reminded that APOLLO2 is a crucial element in industrial chains of both French companies: Electricité de France and AREVA.

[^101]
## Chapter 6 <br> Doppler Effect

The classical Doppler was discovered by the Austrian physicist, Christian Doppler (1803-1853), who in 1842 published an article describing the frequency shift for a wave emitted by a source in motion. Three years later, an experiment confirmed this theory: 15 trumpeters were placed on board a train and some music-lovers experimenters on a train station platform. When the train arrived, the trumpeters continued to play and the emitted sound had a lower pitch after train had passed, as predicted by Doppler. This effect is frequently observed in acoustics, as shown by train and the trumpeters, as well as in electromagnetism, by the "red-shift" measured by astrophysicists, and it is utilized in speed radars. This effect may be used to enable a stationary observer to deduce significant data about a moving target such as its speed and whether it is approaching or receding (Photo 6.1).

However, another so-called nuclear Doppler effect, although less spectacular, is observable in nuclear reactors at the atomic scale, and concerns the relative speed between a neutron and its target nucleus, generally a heavy nuclide. In this case, there is no shift in optical or acoustic frequency, but rather a modification of the resonant cross sections of the target nuclei. This modification is due to the high temperature, and thus, the thermal motion of the target nuclei.

### 6.1 An Intuitive Analysis of the Doppler Effect

As seen previously, the probability of neutron interaction with matter is a function of the total energy of the neutron-target nuclide pair, expressed in the center-ofmass reference frame. Nuclear data libraries generally provide cross sections at a temperature of 0 Kelvin. At that temperature, the target nuclei are "fixed" and the resonance of a given cross section may be represented by a Breit-Wigner formula as a function of the neutron energy $E$ in the center-of-mass reference frame $\left(E=m v^{2} / 2\right.$, where $v$ is the relative velocity of the neutron in the center-of-mass reference frame, $m$ is the reduced mass of the neutron-target system, i.e. $m=m_{n} M /\left(m_{n}+M\right)$,

Photo 6.1 Christian Andreas Doppler (1803-1853) (Public domain)

$v_{r}=|\vec{v}-\vec{V}|$ where $\vec{v}$ is the neutron velocity in the laboratory frame and $\vec{V}$ that of the target nuclide). If $\vec{V}=0$ (theoretical case where the target nuclides are fixed), then $v_{r}=|\vec{v}|$. Supposing that the target nuclei have a speed of $V=|\vec{V}|$, there is a speed shift, and the relative approaching velocity is also shifted and given by $v_{r}=\sqrt{v^{2}+V^{2}-2 v V \cos \theta}$ (in the example given here, $v_{r}>v$ ). The resonance is thus shifted by a constant term. Finally, in the more general and realistic case where each target nucleus has a different velocity, the Maxwell velocity distribution is applied and the resonance widens as the velocity spectrum increases (i.e. as the temperature increases in the case of Brownian motion). Intuitively, the decrease in interaction probability at the resonance energy value stems from the increase in the velocity spectrum of the target nuclei. In the following sections, this intuition will be confirmed by calculating the Doppler broadening. To this end, let us consider a theoretical situation in which all the target nuclei are at 0 K , and each atom thus has the same cross section as a function of energy. Let us next suppose that all of these atoms move in the same direction at the same speed. The cross section, which depends on the total energy of the system, is shifted by the impact of the relative velocity. The resulting cross section is the mean value of the cross sections of all atoms with the same velocity (speed and direction), with each group $f$ atoms having a different shift in speed (Fig. 6.1).

Thus, the effective cross section corresponds to the average that integrates the number of atoms having a given speed. If the temperature increases, the potential speed spectrum widens, resulting in broadening. Furthermore, there are fewer atoms with an energy corresponding exactly to the resonance peak value, which thus decreases.

### 6.2 Effective Interaction Cross Section with "Hot" Matter



The target nuclei are fixed, $T=0 \mathrm{~K}$


The target nuclei have a uniform velocity


The target nuclei each have a different velocity


All of the isotopes have the same apparent effective cross section


The cross section is shifted in energy according to the relative speed


The apparent effective cross section results from the weighted average of all atoms with the same relative speed. The shift has different values and its direction depends on the sign of the relative speed

Fig. 6.1 Empirical analysis of Doppler broadening
We have now seen in previous chapter several models representing the neutronmatter interaction cross section $\sigma(E)$ as a function of neutron energy $E$. The bestknown formalism is the Breit-Wigner formalism, which describes the shape of the cross section at $0 K$ as a function of the nuclear properties of the target nucleus and the incident particle (here, the neutron). In realistic situations, the target nuclei are at a temperature above $0 K$ and in some cases, the thermal agitation of matter (e.g. Brownian motion in gases) cannot be ignored for the cross section; it should be noted that the cross section is given in terms of the incident neutron energy within the center-of-mass reference frame.

### 6.2.1 Distribution of the Target Nuclei Velocities in Matter: The Free Gas Model

At thermal equilibrium, the distribution of $N$ atoms of a free gas at velocity $\vec{V}$ up to $d \vec{V}$ and at temperature $T$ in Kelvin is given by the Maxwell-Boltzmann distribution

Fig. 6.2 Definition of the differential velocity element in spherical coordinates

(which is not strictly valid for a crystal, where chemical bonding must be taken into account since it reduces the degree of freedom of atoms compared to a gas-this situation will be discussed later):

$$
\begin{equation*}
\text { Maxwell-Boltzmann distribution: } \quad N(\vec{V}) d \vec{V}=N\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} e^{-\frac{M}{2 k T} V^{2}} d \vec{V} \tag{6.1}
\end{equation*}
$$

Note that $d \vec{V}$ is a vector differential element, hence a velocity "volume" centered on $\vec{V}$, denoted in some publications as $d^{3} \vec{V}$. In spherical coordinates, the differential volume element is given by: $d \vec{V}=V^{2} d V \sin \theta d \theta d \varphi$ (Fig. 6.2).

### 6.2.2 Definition of the Effective Cross Section

The interaction rate of $n(v)$ neutrons of speed $v$ (in the laboratory frame) with $N(V)$ target nuclei of speed $V$ (in the laboratory frame) is given by:

$$
R(\vec{v}, \vec{V})=n(\vec{v}) \sigma(|\vec{v}-\vec{V}|) N(\vec{V})
$$

The relative speed term is used because the cross section depends on the relative speed of the neutron in the center-of-mass frame. Thus, the total reaction rate for neutrons with speed $v$, given by integration over the target atoms with speed $V$, is:

$$
R(\vec{v})=n(\vec{v}) \int_{\vec{V}}|\vec{v}-\vec{V}| \sigma(|\vec{v}-\vec{V}|) N(\vec{V}) d \vec{V}
$$

The reaction rate can also be written as:

$$
R(\vec{v})=n(\vec{v}) v \bar{\sigma}(v) N
$$

Where $N$ is the number of target nuclei and $\bar{\sigma}(v)$ is the effective cross section for a neutron with speed $v$. The effective cross section is thus:

$$
\begin{equation*}
\text { Effective cross section: } \quad \bar{\sigma}=\frac{1}{N v} \int_{\vec{V}}|\vec{v}-\vec{V}| \sigma(|\vec{v}-\vec{V}|) N(\vec{V}) d \vec{V} \tag{6.2}
\end{equation*}
$$

### 6.2.3 Cross Section Inversely Proportional to Velocity

Let us consider the special case of a microscopic cross section varying as $1 / v$ :

$$
\sigma(|\vec{v}-\vec{V}|)=\sigma_{0} \frac{v_{0}}{(v-V)}
$$

By substitution in the previous equation, the velocities cancel out in the integral:
$1 / v$ cross section broadened by Doppler effect:

$$
\begin{equation*}
\bar{\sigma}=\frac{1}{N v} \int_{\vec{V}} \sigma_{0} v_{0} N(\vec{V}) d \vec{V}=\sigma_{0} \frac{v_{0}}{v} \tag{6.3}
\end{equation*}
$$

Hence, a pure $1 / v$ cross section is not temperature-dependent and displays no Doppler effect. The particular case of the ${ }^{10} B$ cross section, which varies as $1 / v$ throughout the entire spectrum (Fig. 6.3), provides a good example.

### 6.2.4 Constant Cross Section

The broadening of a constant cross section (as is the case for the scattering cross section of several light isotopes such as hydrogen or carbon over a large energy range) is particularly interesting. Let us begin with the definition of the effective cross section:

$$
\bar{\sigma} \equiv \frac{1}{N v} \int_{\vec{V}}|\vec{v}-\vec{V}| \underbrace{\sigma(|\vec{v}-\vec{V}|)}_{\sigma_{0}} N(\vec{V}) d \vec{V}=\frac{\sigma_{0}}{v} \int_{V=0}^{V=+\infty}|\vec{v}-\vec{V}|\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} e^{-\frac{M}{2 k T} V^{2}} d \vec{V}
$$

The vector differential element of velocity is given by: $d \vec{V}=V^{2} d V \sin \theta d \theta d \varphi$. Defining $\theta$ as the angle between the velocities of the neutron and the target nucleus, and choosing the $z$ axis as the direction of the incident neutron, we get:


Fig. 6.3 Doppler broadening of the $(n, \alpha)$ cross section of ${ }_{5}^{10} B$ (adapted from the NJOY documentation)

$$
|\vec{v}-\vec{V}|=\sqrt{v^{2}+V^{2}-2 v V \cos \theta}
$$

The standard integration variable used is $\mu=\cos \theta$ (Barjon 1993, p. 72):

$$
\begin{aligned}
\bar{\sigma} & =\frac{\sigma_{0}}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} \int_{V=0}^{V=+\infty} \int_{0}^{2 \pi} d \varphi \int_{\theta=0}^{\theta=\pi} \sqrt{v^{2}+V^{2}-2 v V \cos \theta} e^{-\frac{M}{2 k T} V^{2}} V^{2} d V \sin \theta d \theta \\
& =\frac{\sigma_{0}}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} 2 \pi \int_{V=0}^{V=+\infty \mu=+1} \int_{\mu=-1} \sqrt{v^{2}+V^{2}-2 v V \mu} e^{-\frac{M}{2 k T} V^{2}} V^{2} d V d \mu \\
& =\frac{\sigma_{0}}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} 2 \pi \int_{V=0}^{V=+\infty} e^{-\frac{M}{2 k T} V^{2}} V^{2} d V(-\frac{2}{3} \frac{1}{2 v V} \underbrace{\left[\left(v^{2}+V^{2}-2 v V \mu\right)^{\frac{3}{2}}\right]_{-1}^{+1}}_{(V-v)^{\frac{6}{2}-(V+v)^{\frac{6}{2}}}})
\end{aligned}
$$

The integrated term depends on the sign of the $V-v$ difference:

$$
\left(v^{2}+V^{2}-2 v V \mu\right)^{\frac{3}{2}}=\left\{\begin{array}{lll}
(V-v)^{3}-(V+v)^{3}=-2 v\left(V^{2}+3 v^{2}\right) & \text { if } \quad V>v \\
(v-V)^{3}-(V+v)^{3}=-2 V\left(v^{2}+3 V^{2}\right) & \text { if } \quad V<v
\end{array}\right.
$$

Thus:
$\bar{\sigma}=\frac{\sigma_{0}}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} 2 \pi \int_{V=0}^{V=v} e^{-\frac{M}{2 k T} V^{2}} V^{2}\left(2 v+\frac{2 V^{2}}{3 v}\right) d V+\int_{V=v}^{V=+\infty} e^{-\frac{M}{2 k T} V^{2}} V^{2}\left(2 V+\frac{2 v^{2}}{3 V}\right) d V$
With a few algebraic operations, the different moments $\left\langle V^{n}\right\rangle$ may be evaluated and weighted by the function $\exp \left(-M V^{2} /(2 k T)\right)$ using the following change in variable $M V^{2} /(2 k T) \equiv \alpha^{2} V^{2}=x$, and defining $\alpha \equiv \sqrt{M /(2 k T)}$ to simplify the expressions:

$$
\left\langle V^{n}\right\rangle \equiv \int_{V=0}^{V=+\infty} e^{-\frac{M}{2 k T} V^{2}} V^{n} d V=\int_{x=0}^{x=+\infty} e^{-x} \frac{x^{\frac{n}{2}}}{\alpha^{n}} \frac{1}{2 \alpha} x^{-\frac{1}{2}} d x=\frac{1}{2 \alpha^{n+1}} \Gamma\left(\frac{n+1}{2}\right)
$$

As for the partial integrals, the error function $\operatorname{erf}(x)=\frac{2}{\sqrt{\pi}} \int_{0}^{+\infty} e^{-t^{2}} d t$ is sought for using the variable change $M V^{2} /(2 k T) \equiv \alpha^{2} V^{2}=y^{2}$

$$
I E_{n}(v) \equiv \int_{V=0}^{V=v} e^{-\frac{M}{2 k T} V^{2}} V^{n} d V=\int_{y=0}^{y=\alpha v} e^{-y^{2}} \frac{y^{n}}{\alpha^{n+1}} d y
$$

which, when integrated by parts, leads to a recurrence relation that couples the integral terms $n$ and $n+2$ :

$$
\begin{aligned}
I E_{n}(v) & \equiv \int_{y=0}^{y=\alpha v} e^{-y^{2}} \frac{y^{n}}{\alpha^{n+1}} d y=\frac{1}{\alpha^{n+1}}\left(\left[e^{-y^{2}} \frac{y^{n+1}}{n+1}\right]_{0}^{\alpha v}-\int_{y=0}^{y=\alpha v}-2 y e^{-y^{2}} \frac{y^{n+1}}{n+1} d y\right) \\
& =\frac{v^{n+1}}{(n+1)} e^{-\alpha^{2} v^{2}}+2 \frac{\alpha^{2}}{n+1} I E_{n+2}(v)
\end{aligned}
$$

and the recurrence is initialized by:

$$
I E_{0}(v) \equiv \int_{y=0}^{y=\alpha v} e^{-y^{2}} \frac{1}{\alpha} d y=\frac{\sqrt{\pi}}{2 \alpha} \operatorname{erf}(\alpha v) \text { and } I E_{1}(v) \equiv \int_{y=0}^{y=\alpha v} e^{-y^{2}} \frac{y}{\alpha^{2}} d y=\frac{1}{2 \alpha^{2}}\left(1-e^{-\alpha^{2} v^{2}}\right)
$$

Hence:

$$
\left\{\begin{array}{l}
I E_{2}(v)=\frac{\sqrt{\pi}}{4 \alpha^{3}} \operatorname{erf}(\alpha v)-\frac{v}{2 \alpha^{2}} e^{-\alpha^{2} v^{2}} \\
I E_{3}(v) \equiv \frac{1}{2 \alpha^{4}}\left(1-e^{-\alpha^{2} v^{2}}\right)-\frac{v^{2}}{2 \alpha^{2}} e^{-\alpha^{2} v^{2}} \\
I E_{4}(v)=\frac{3 \sqrt{\pi}}{8 \alpha^{5}} \operatorname{erf}(\alpha v)-\frac{3 v}{4 \alpha^{4}} e^{-\alpha^{2} v^{2}}-\frac{v^{3}}{2 \alpha^{2}} e^{-\alpha^{2} v^{2}}
\end{array}\right.
$$

The integrals between $[v,+\infty$ [ are obtained by the difference:

$$
I F_{n}(v) \equiv \int_{V=v}^{V=+\infty} v e^{-\frac{M}{2 k T} V^{2}} V^{n} d V=\left\langle V^{n}\right\rangle-I E_{n}(v)
$$

These terms may be combined to give:

$$
\begin{gathered}
\bar{\sigma}=\frac{\sigma_{0}}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} 2 \pi\left[2 v I E_{2}(v)+\frac{2}{3 v} I E_{4}(v)+2 I F_{3}(v)+\frac{2 v^{2}}{3} I F_{1}(v)\right] \\
\bar{\sigma}=\frac{\sigma_{0}}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} 2 \pi\left[\begin{array}{l}
2 v\left(\frac{\sqrt{\pi}}{4 \alpha^{3}} \operatorname{erf}(\alpha v)-\frac{v}{2 \alpha^{2}} e^{-\alpha^{2} v^{2}}\right) \\
+\frac{2}{3 v}\left(\frac{3 \sqrt{\pi}}{8 \alpha^{5}} \operatorname{erf}(\alpha v)-\frac{3 v}{4 \alpha^{4}} e^{-\alpha^{2} v^{2}}-\frac{v^{3}}{2 \alpha^{2}} e^{-\alpha^{2} v^{2}}\right) \\
+2\left(\frac{1}{2 \alpha^{4}} \Gamma(2)-\frac{1}{2 \alpha^{4}}\left(1-e^{-\alpha^{2} v^{2}}\right)+\frac{v^{2}}{2 \alpha^{2}} e^{-\alpha^{2} v^{2}}\right) \\
+\frac{2 v^{2}}{3}\left(\frac{1}{2 \alpha^{2}} \Gamma(1)-\frac{1}{2 \alpha^{2}}\left(1-e^{-\alpha^{2} v^{2}}\right)\right)
\end{array}\right]
\end{gathered}
$$

which can be simplified algebraically as:

$$
\bar{\sigma}(v)=\sigma_{0}\left[\left(1+\frac{1}{2 \alpha^{2} v^{2}}\right) \operatorname{erf}(\alpha v)+\frac{1}{\alpha v} \frac{1}{\sqrt{\pi}} e^{-\alpha^{2} v^{2}}\right]
$$

The expression is then written in terms of energy using the incident neutron kinetic energy $E=m v^{2} / 2$, i.e. $\alpha v_{[-]}=\sqrt{M v /(2 k T)}=\sqrt{A E /(k T)}$ with $A=M / m$ :

Constant cross section broadened by the Doppler effect:

It is observed that when $x \equiv A E /(k T) \gg 1$, since $\lim _{x \rightarrow+\infty} \operatorname{erf}(x)=1$ and the exponential term tends to 0 , the cross section tends to the original constant cross section $\sigma_{0}$ when varying with energy. However, when $x \ll 1$, then $\operatorname{erf}(x) \approx 2 x /$ $\sqrt{\pi}$ and the exponential tends to 1 .

$$
\bar{\sigma}(E) \approx \sigma_{0} \frac{2}{\sqrt{\pi}} \sqrt{\frac{k T}{A E}}=\sigma_{0} \frac{2}{\sqrt{\pi}} \sqrt{\frac{2 k T}{M v^{2}}}=\sigma_{0} \frac{\bar{V}}{v}
$$

where $\bar{V}=\frac{2}{\sqrt{\pi}} \sqrt{\frac{2 k T}{M}}=\frac{2}{\sqrt{\pi}} V_{T}$ is the mean speed of the target nuclei at temperature $T$ and with $V_{T}$ being the most probable speed. At low energy, a $1 / v$ shape is observed


Fig. 6.4 Doppler broadening of the total cross section of ${ }_{6}^{12} C$ (from the NJOY documentation)
and this characteristic becomes more prominent as temperature increases $\left({ }_{6}^{12} C\right.$ case, Fig. 6.4).

### 6.3 Generalized Doppler Broadening: Bethe-Placzek Formula

By introducing the speed distribution of the target nuclei into the effective cross section expression, the following is obtained:

$$
\bar{\sigma}=\frac{1}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} \int_{\vec{V}}|\vec{v}-\vec{V}| \sigma(|\vec{v}-\vec{V}|) e^{-\frac{M}{2 k T} V^{2}} d \vec{V}
$$

Let the relative velocity vector be $\vec{v}_{r}=\vec{V}-\vec{v}$, enabling the target velocity to be computed in terms of the relative velocity: $\vec{V}=\vec{v}+\vec{v}_{r}$ with the differential element $d \vec{v}_{r}=d \vec{V}$ since $\vec{v}$ is constant in the integral (Fig. 6.5).

The effective cross section is then expressed in terms of the relative velocity, which becomes the sole remaining integration variable after efficient vector simplification:

Fig. 6.5 Velocity vector triangle


$$
\bar{\sigma}=\frac{1}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} \int_{\vec{v}_{R}} v_{r} \sigma\left(v_{r}\right) e^{-\frac{M}{2 k T}\left|\vec{v}+\vec{v}_{r}\right|^{2}} d \vec{v}_{r}
$$

By composition of vectors: $\quad\left|\vec{v}+\vec{v}_{r}\right|^{2}=v^{2}+v_{r}^{2}+2 v v_{r} \cos \left(\vec{v}, \vec{v}_{r}\right)=$ $v^{2}+v_{r}^{2}+2 v v_{r} \cos \theta$

Hence $\quad \bar{\sigma}=\frac{1}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} \int_{\vec{v}_{r}} v_{r} \sigma\left(v_{r}\right) e^{-\frac{M}{2 k T}\left(v^{2}+v_{r}^{2}\right)} e^{-\frac{M}{2 k T} 2 v v_{r} \cos \theta} d \vec{v}_{r}$
In spherical coordinates, with the $z$ axis in the $\vec{v}$ direction, the relative velocity differential element is written as $d \vec{v}_{r}=v_{r}^{2} d v_{r} \sin \theta d \theta d \varphi$, leading to:

$$
\bar{\sigma}=\frac{1}{v}\left(\frac{M}{2 \pi k T}\right)^{\frac{3}{2}} \int_{0}^{2 \pi} d \varphi \int_{0}^{+\infty} v_{r}^{3} \sigma\left(v_{r}\right) e^{-\frac{M}{2 k T}\left(v^{2}+v_{r}^{2}\right)} \int_{0}^{\pi} e^{-\frac{M}{2 k T} 2 v v_{r} \cos \theta} \sin \theta d \theta d v_{r}
$$

The integration over $\varphi$ is obvious, while that over $\theta$ requires a change of variable such that $\mu=\cos \theta$, i.e. $d \mu=-\sin \theta d \theta$ giving the following:

$$
\bar{\sigma}=\frac{1}{v}\left(\frac{M}{k T}\right)^{\frac{3}{2}} \frac{1}{\sqrt{2 \pi}} \int_{0}^{+\infty} v_{r}^{3} \sigma\left(v_{r}\right) e^{-\frac{M}{2 k T}\left(v^{2}+v_{r}^{2}\right)} \int_{-1}^{+1} e^{-\frac{M}{2 k T} 2 v v_{r} \mu} d \mu d v_{r}
$$

After computation of the integral term with respect to $d \mu$ :

$$
\bar{\sigma}=\frac{1}{v}\left(\frac{M}{k T}\right)^{\frac{3}{2}} \frac{1}{\sqrt{2 \pi}} \int_{0}^{+\infty} v_{r}^{3} \sigma\left(v_{r}\right) e^{-\frac{M}{2 k T}\left(v^{2}+v_{r}^{2}\right)}\left[\frac{e^{-\frac{M}{2 k T} 2 v v_{r}}-e^{\frac{M}{2 k T} 2 v v_{r}}}{-\frac{M}{2 k T} 2 v v_{r}}\right] d v_{r}
$$

It may be seen that the resulting expression is composed of perfect squares, and by simplifying it, the Bethe-Placzek equation in velocity is obtained:

Bethe-Placzek equation in velocity:

$$
\begin{equation*}
\bar{\sigma}=\frac{1}{v^{2}} \sqrt{\frac{M}{2 \pi k T}} \int_{0}^{+\infty} v_{r}^{2} \sigma\left(v_{r}\right)\left[e^{-\frac{M}{2 k T}\left(v-v_{r}\right)^{2}}-e^{-\frac{M}{2 k T}\left(v+v_{r}\right)^{2}}\right] d v_{r} \tag{6.5}
\end{equation*}
$$



Hans Bethe (left) and George Placzek (right) (Public domain)

This equation is also presented in certain publications by introducing a velocity corresponding to twice the thermal energy $k T: v_{t h}=\sqrt{k T / M}$, thus giving the form:

$$
\bar{\sigma}=\frac{1}{\sqrt{2 \pi} v_{t h} v^{2}} \int_{0}^{+\infty} v_{r}^{2} \sigma\left(v_{r}\right)\left[e^{-\frac{1}{2 v_{t h}^{2}}\left(v-v_{r}\right)^{2}}-e^{-\frac{1}{2 v_{t h} h^{2}}\left(v+v_{r}\right)^{2}}\right] d v_{r}
$$

At this stage, there is no simplifying approximation and the equation is exact under the hypothesis that the distribution of target nuclei is a Maxwellian distribution. The latter implies a free gas model with no interaction, save for elastic collisions. This equation is transformed to obtain energy as a variable. Let $E$ be the neutron energy in the laboratory frame $\left(E=m v^{2} / 2\right)$ and $\varepsilon$ the neutron energy in the center-of-mass frame $\left(\varepsilon=m v_{r}^{2} / 2\right)$, which gives:

$$
\bar{\sigma}=\left(\frac{m}{2 E}\right) \sqrt{\frac{M}{2 \pi k T}} \int_{0}^{+\infty} \frac{2 \varepsilon}{m} \sigma(\varepsilon)\left[e^{-\frac{M}{2 k T}\left(\sqrt{\frac{2 E}{m}}-\sqrt{\frac{\varepsilon \varepsilon}{m}}\right)^{2}}-e^{-\frac{M}{2 k T}\left(\sqrt{\frac{2 E}{m}}+\sqrt{\frac{\sqrt{E}}{m}}\right)^{2}}\right] \frac{d \varepsilon}{\sqrt{2 \varepsilon m}}
$$

For a free gas, the Bethe-Placzek equation in energy is obtained with $A=M / m$ (Fig. 6.6):

Bethe-Placzek equation in energy:

$$
\begin{equation*}
\bar{\sigma}=\frac{1}{E} \sqrt{\frac{A}{4 \pi k T}} \int_{0}^{+\infty} \sqrt{\varepsilon} \sigma(\varepsilon)\left[e^{-\frac{A}{k T}(\sqrt{E}-\sqrt{\varepsilon})^{2}}-e^{-\frac{A}{k T}(\sqrt{E}+\sqrt{\varepsilon})^{2}}\right] d \varepsilon \tag{6.6}
\end{equation*}
$$



Fig. 6.6 Doppler broadening of the $(n, \gamma)$ cross section of ${ }_{94}^{240} \mathrm{Pu}$ (from the NJOY documentation)

In the case of a cubic crystal lattice in which atoms are bounded by the lattice energy, Willis Lamb ${ }^{1}$ (in 1939) established that the previous form was still valid using an effective temperature $T_{\text {eff }}$ instead of $T$. This temperature is given by (Fröhner 2000, p. 72):

$$
T_{e f f}=T\left(\frac{T}{\theta_{D}}\right)^{3} \frac{3}{2} \int_{0}^{\frac{\theta_{D}}{T}} x^{3} \operatorname{coth}\left(\frac{x}{2}\right) d x \approx T\left(1+\frac{1}{20}\left(\frac{\theta_{D}}{T}\right)^{2}-\ldots\right)
$$

where $\theta_{D}$ is the Debye ${ }^{2}$ temperature of the crystal (Dresner 1960, p. 33; Mazenko 2000, p. 488). For power reactors with uranium fuel, the true temperature is much higher than the Debye temperature, and is taken as the effective temperature of the

[^102]medium. This approximation is not justified for carbon structures as in French Uranium Naturel Graphite Gaz (UNGG) reactors. The effective temperature will be discussed later.

### 6.4 Doppler Broadening of a Breit-Wigner Cross Section

### 6.4.1 Overview of the Breit-Wigner Formalism

The Breit-Wigner formalism is based on understanding of the decay of the intermediate nucleus. The latter is formed during the interaction of an incident particle with a target nucleus. The neutron energy from the Breit-Wigner equation is expressed in the center-of-mass frame $\varepsilon=m v_{r}^{2} / 2$. Breit and Wigner described the behavior of the cross section in the vicinity of a resonance using a first-level formula for neutrons with zero angular momentum:

$$
\sigma_{n, \gamma}(\varepsilon)=\underbrace{4 \pi \AA^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}}}_{\sigma_{n, \gamma} 0} \frac{1}{1+\left(\frac{2\left(\varepsilon-E_{0}\right)}{\Gamma}\right)^{2}}=\sigma_{n, \gamma 0} \frac{1}{1+x^{2}}
$$

with

$$
\sigma_{n, \gamma 0}=\sigma_{t 0}(\varepsilon) \frac{\Gamma_{\gamma}}{\Gamma}=4 \pi \lambda^{2} g \frac{\Gamma_{n} \Gamma_{\gamma}}{\Gamma^{2}}
$$



Peter Debye (Public domain).

Fig. 6.7 A Breit-Wigner cross section in the vicinity of a resonance


The neutron width of resonant scattering $\Gamma_{n}$, of radiative capture $\Gamma_{\gamma}$ and of fission $\Gamma_{f}$ are defined. Experiments have shown that $\Gamma_{n}$ depends on energy $\varepsilon$ according to the following equation (Fig. 6.7):

$$
\Gamma_{n}(\varepsilon)=\Gamma_{n}\left(E_{0}\right) \sqrt{\frac{\varepsilon}{E_{0}}}
$$

The sum of the partial widths amounts to $\Gamma$, the width of the total resonance. Close to the resonance, this equation is simplified by assuming that $\sigma_{0}$ is constant. Nevertheless, for the rest of this chapter, the term with a square root in energy is kept as it translates the fact that the cross section has a $1 / v$ form at low energies. Thus:

$$
\sigma_{(n, \gamma)}(\varepsilon)=\sigma_{0} \frac{\Gamma_{i}}{\Gamma} \sqrt{\frac{E_{0}}{\varepsilon}} \frac{1}{1+\left(\frac{2\left(\varepsilon-E_{0}\right)}{\Gamma}\right)^{2}}
$$

The term $\sqrt{E_{0} / \varepsilon}$ shows the $1 / v$ tendency of the cross section far from the resonance at low energy:

$$
\sigma_{t 0}(\varepsilon)=4 \pi \hbar^{2} g \frac{\Gamma_{n}\left(E_{0}\right) \sqrt{\frac{\varepsilon}{E_{0}}}}{\Gamma}=4 \pi \frac{\hbar^{2}}{2 \mu \varepsilon} g \sqrt{\frac{\varepsilon}{E_{0}}}=\underbrace{2 \pi \frac{h^{2}}{\mu E_{0}} g \Gamma_{n}\left(E_{0}\right)}_{\sigma_{0}} \sqrt{\frac{E_{0}}{\varepsilon}}=\sigma_{0} \sqrt{\frac{E_{0}}{\varepsilon}}
$$

hence: $\quad \sigma_{n, \gamma 0}=\sigma_{t 0}(\varepsilon) \frac{\Gamma_{\gamma}}{\Gamma}=\sigma_{0} \sqrt{\frac{E_{0}}{\varepsilon}} \frac{\Gamma_{\gamma}}{\Gamma}$
For an energy much greater than that of the resonance ( $\varepsilon \gg E_{0}$ ), the asymptotic behavior of a resonance can be induced as the inverse of the energy variable to the power of $5 / 2$ :

$$
\sigma_{(n, \gamma)}(\varepsilon)=\sigma_{0} \frac{\Gamma_{i}}{\Gamma} \sqrt{\frac{E_{0}}{\varepsilon}} \frac{1}{1+\left(\frac{2\left(\varepsilon-E_{0}\right)}{\Gamma}\right)^{2}} \approx \sigma_{0} \frac{\Gamma_{i} \Gamma \sqrt{E_{0}}}{4 \varepsilon^{\frac{5}{2}}}
$$

### 6.4.2 Voigt's Formula

The Bethe-Placzek equation in energy is transformed by introducing the BreitWigner model:

$$
\bar{\sigma} \approx \frac{\sigma_{0}}{\sqrt{\pi}} \frac{\Gamma_{i}}{\Gamma} \frac{E_{0}}{E} \sqrt{\frac{A}{4 k T E_{0}}} \int_{0}^{+\infty} \frac{e^{-\frac{A}{k T}(\sqrt{\varepsilon}-\sqrt{E})^{2}}-e^{-\frac{A}{k T}(\sqrt{\varepsilon}+\sqrt{E})^{2}}}{4\left(\frac{\varepsilon-E_{0}}{\Gamma}\right)^{2}+1} d \varepsilon
$$

The following is a simplification based on physical considerations: the neutrons are generally at energy values higher than the thermal energy, i.e. $E \gg k T$ and $E \approx \varepsilon$. This hypothesis leads to three simplifications: in the second exponential term, the following can be written:

$$
(\sqrt{E}+\sqrt{\varepsilon})^{2} \approx 4 E \gg k T
$$

that is, a very small exponential term. On the other hand, in the first exponential, $(\sqrt{E}-\sqrt{\varepsilon})^{2} \approx 0$, i.e. an exponential value close to 1 . The second exponential term can be neglected compared to the first. Furthermore, with a Taylor expansion:

$$
\sqrt{\varepsilon}=\sqrt{E+(\varepsilon-E)}=\sqrt{E} \sqrt{1+\frac{\varepsilon-E}{E}} \approx \sqrt{E}\left(1+\frac{\varepsilon-E}{2 E}\right)
$$

thereby leading to a simplification of the first exponential term: $e^{-\frac{A}{k T} \frac{(\varepsilon-E)^{2}}{4 E}}$. Finally, in the integral term, $\sqrt{\varepsilon} / E \approx 1 / \sqrt{E_{0}}$, which equates to the fact that $\varepsilon$ is very close to $E$, this is the very hypothesis which was used in the previous expansion. Hence, only energy values close to $E_{0}$ contribute to the integral term. On moving away from $E_{0}$, the Breit-Wigner model is obviously no longer appropriate since either there is the influence of another resonance (of energy $E_{1}$ ), the cross section is constant (potential cross section), or at very low energies there is a $1 / v$ tendency. The general form of the cross section is the sum of the different resonances of Breit-Wigner cross sections (with an interference term between resonances) and the potential cross section $\left(4 \pi R^{2}\right)$. Finally, the cross section is defined with an improper integral over

Photo 6.2 Woldemar Voigt (1850-1919): A precursor in the field of relativity theory (Public domain)

energy called the Voigt formula, ${ }^{3}$ which derives from his work on the broadening of Gaussian distribution and is widely tabulated in the literature (Stacey 2001, p. 115; Barjon 1993, p. 81; Foderaro 1971, p. 515); see also. ${ }^{4}$

$$
\begin{equation*}
\text { Voigt's formula: } \quad \bar{\sigma} \approx \sigma_{0} \frac{\Gamma_{i}}{\Gamma} \frac{1}{\sqrt{\pi}} \sqrt{\frac{A}{4 k T E_{0}}} \int_{0}^{+\infty} \frac{e^{-\frac{1}{4 k T E_{0}}}(\varepsilon-E)^{2}}{4\left(\frac{\varepsilon-E_{0}}{\Gamma}\right)^{2}+1} d \varepsilon \tag{6.7}
\end{equation*}
$$

It should be noted that the physical hypotheses applied earlier render the foregoing formula inappropriate for resonances at low energies (in the thermal energy range).

These hypotheses are too often overlooked and Voigt's formula is applied to all the resonances, even those at low energies (e.g. for certain even isotopes of

[^103]plutonium). (Duderstatd and Hamilton 1976) gives the example of the 0.296 eV resonance of ${ }_{94}^{239} \mathrm{Pu}$ where applying Voigt's formula at $2000^{\circ} \mathrm{C}$ leads to a discrepancy of $50 \%$ compared to the exact formula. Let us set the following:
\[

$$
\begin{equation*}
\text { Doppler width: } \quad \Delta \equiv \sqrt{\frac{4 k T E_{0}}{A}} \tag{6.8}
\end{equation*}
$$

\]

widely called the Doppler width. The cross section is written using the previous variable:

$$
\bar{\sigma} \approx \sigma_{0} \frac{\Gamma_{i}}{\Gamma} \frac{1}{\sqrt{\pi}} \frac{1}{\Delta} \int_{0}^{+\infty} \frac{e^{-\frac{1}{4 \Delta^{2}}(\varepsilon-E)^{2}}}{4\left(\frac{\varepsilon-E_{0}}{\Gamma}\right)^{2}+1} d \varepsilon
$$

The dimensionless energy variable is then set as: $x=2\left(E-E_{0}\right) / \Gamma$, i.e. $E=E_{0}+x \frac{\Gamma}{2}$ :

$$
\bar{\sigma} \approx \sigma_{0} \frac{\Gamma_{i}}{\Gamma} \frac{1}{\sqrt{\pi}} \frac{1}{\Delta} \int_{0}^{+\infty} \frac{e^{-\frac{1}{4}\left(\frac{\Gamma}{\Delta}\right)^{2}\left(2 \frac{\varepsilon-E_{0}}{\Gamma}-x\right)^{2}}}{4\left(\frac{\varepsilon-E_{0}}{\Gamma}\right)^{2}+1} d \varepsilon
$$

Finally, the reduced variable for integration is set as: $y=2 \frac{\varepsilon-E_{0}}{\Gamma}$, i.e. $d \varepsilon=\frac{\Gamma}{2} d y$ which varies from $-2 \frac{E_{0}}{\Gamma}$ to $+\infty$.

Hence, the effective cross section is expressed as:

$$
\bar{\sigma} \approx \sigma_{0} \frac{\Gamma_{i}}{\Gamma} \frac{1}{2 \sqrt{\pi}} \frac{\Gamma}{\Delta} \int_{-\frac{E_{0}}{T}}^{+\infty} \frac{e^{-\frac{1}{4}\left(\frac{\Gamma}{4}\right)^{2}(y-x)^{2}}}{y^{2}+1} d y
$$

Let us now examine a narrow resonance, with the Narrow Resonance approximation, i.e. $E_{0} \gg \Gamma$. This hypothesis allows integration to be extended up to $-\infty$. Finally, the dimensionless number $\xi=\Gamma / \Delta$ is used to deduce the first Voigt function $\Psi$ :

$$
\bar{\sigma} \approx \sigma_{0} \frac{\Gamma_{i}}{\Gamma} \Psi(x, \xi)=\sigma_{0} \frac{\Gamma_{i}}{\Gamma}\left[\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4}(x-y)^{2}}}{y^{2}+1} d y\right]
$$

The Voigt function $\Psi$ is defined as:

$$
\begin{equation*}
\text { First Voigt function: } \quad \Psi(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4}(x-y)^{2}}}{y^{2}+1} d y \tag{6.9}
\end{equation*}
$$

The equation is independent of the target nucleus thanks to the use of dimensionless parameters. This function is the convolution of a Breit-Wigner function by a Gaussian distribution. This integral cannot be computed analytically and has been calculated by numerical methods since the 1940s, and by computer as soon as feasible. The results have been tabulated for a wide range of values of $x$ and $\xi$. As temperature $T$ tends towards 0 , the target nuclei are no longer in motion, and $\vec{v}_{R}=\vec{V}-\vec{v}$ tends towards $v$. Hence, $\varepsilon$ tends towards $E$ and $y$ tends towards $x$. We may thus write:

$$
\begin{aligned}
\lim _{T \rightarrow 0 K}(\Psi(\xi, x)) & =\lim _{T \rightarrow 0 K}\left(\frac{\xi}{2 \sqrt{\pi}} \frac{1}{1+x^{2}} \int_{-\infty}^{+\infty} e^{-\frac{\xi^{2}}{4}(x-y)^{2}} d y\right) \\
& =\frac{1}{\sqrt{\pi}} \frac{1}{1+x^{2}} \int_{-\infty}^{+\infty} e^{-u^{2}} d u
\end{aligned}
$$

However, the integral of a Gauss distribution from $-\infty$ to $+\infty$ is equal to $\Gamma(1 / 2)=\sqrt{\pi}$. Thus, the following is deduced:

$$
\lim _{T \rightarrow 0 K} \bar{\sigma}(x)=\sigma_{0} \frac{\Gamma_{i}}{\Gamma} \frac{1}{1+x^{2}}
$$

To conclude, the Voigt cross section, although the simplification, tends towards the Breit-Wigner cross section for very low temperature values, which was to be expected from a physics point of view and based on the Breit-Wigner model. High temperatures correspond to cases where $\xi$ is close to 0 . Therefore, the exponential is close to 1 and almost constant, equal to $\exp \left(-\xi^{2} x^{2} / 4\right)$. This term is removed from the integration term:

$$
\begin{aligned}
\lim _{T \rightarrow \infty}(\Psi(\xi, x)) & =\lim _{\xi \rightarrow 0}\left(\frac{\xi}{2 \sqrt{\pi}} e^{-\frac{\xi^{2}}{4} x^{2}} \int_{-\infty}^{+\infty} \frac{1}{1+y^{2}} d y\right) \\
& =\left(\int_{-\infty}^{+\infty} \frac{1}{1+y^{2}} d y\right) \lim _{\xi \rightarrow 0}\left(\frac{\xi}{2 \sqrt{\pi}} e^{-\frac{\xi^{2}}{4} x^{2}}\right)
\end{aligned}
$$

Using $x=2 \frac{E-E_{0}}{\Gamma}, \xi=\frac{\Gamma}{\Delta}$ and finally, $\int_{-\infty}^{+\infty} \frac{1}{1+y^{2}} d y=\pi$, we obtain the following:

$$
\bar{\sigma}=\sigma_{0} \frac{\sqrt{\pi}}{2} \frac{\Gamma_{i}}{\Delta} e^{-\frac{\left(E-E_{0}\right)^{2}}{\Delta^{2}}}
$$



Fig. 6.8 Doppler broadening at very high temperature for the $(n, \gamma)$ resonance of ${ }_{94}^{240} P u$ at 20 MeV (adapted from the NJOY documentation)

At high temperatures, the Voigt cross section tends to a Gauss distribution centered on $E_{0}$ and of width $\Delta$. Hence, the term natural Doppler width for $\Delta$. It should be noted that this width does not depend on $\Gamma$ (Fig. 6.8).

It can immediately be seen that the function $\Psi$ is strictly positive since it is the integral of strictly positive functions for any value of $x$. Furthermore, it is even with respect to $x$ and has an extremum (peak value) at $x=0$. At infinity it tends towards 0 .

$$
\begin{aligned}
\lim _{x \rightarrow \infty}(\Psi(\xi, x)) & =\lim _{x \rightarrow \infty}\left(\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4}(x-y)^{2}}}{1+y^{2}} d y\right) \\
& =\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{1}{1+y^{2}} \lim _{x \rightarrow \infty}\left(e^{-\frac{\xi^{2}}{4}(x-y)^{2}}\right) d y=0
\end{aligned}
$$

The Voigt function has an interesting property: its integral is conserved with respect to energy. Indeed, it can be seen that $\operatorname{Area}(T)=\int_{-\infty}^{+\infty} \bar{\sigma}(x, T) d E$ simplifies to:

$$
\operatorname{Area}(T)=\int_{-\infty}^{+\infty} \sigma_{0} \frac{\Gamma_{i}}{\Gamma}\left[\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi 2}{4}(y-x)^{2}}}{y^{2}+1} d y\right] d E
$$

The two integrals are interchanged and then, using the reduced energy, $x=2\left(E-E_{0}\right) / \Gamma$, i.e. $d E=\Gamma d x / 2$, we obtain the following:

$$
\begin{aligned}
\operatorname{Area}(T) & =\sigma_{0} \frac{\Gamma_{i}}{\Gamma} \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{1}{y^{2}+1}\left(\int_{-\infty}^{+\infty} e^{-\frac{\xi^{2}}{4}(y-x)^{2}} \frac{\Gamma}{2} d x\right) d y \\
& =\sigma_{0} \Gamma_{i} \frac{\xi}{4 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{1}{y^{2}+1}\left(\int_{-\infty}^{+\infty} e^{-u^{2}} \frac{2}{\xi} d u\right) d y
\end{aligned}
$$

It may then be seen that the integral $A$ is constant and independent of temperature, which is not evident on first grounds a priori (Fig. 6.9).

$$
\text { Area }=\frac{\sigma_{0} \Gamma_{i}}{2} \int_{-\infty}^{+\infty} \frac{1}{y^{2}+1} d y=\frac{\sigma_{0} \Gamma_{i}}{2}[\operatorname{Arctg}(y)]_{-\infty}^{+\infty}=\frac{\pi}{2} \sigma_{0} \Gamma_{i}
$$

To conclude, the area under the cross section curve is conserved when temperature varies. Hence, if the maximum of the resonance decreases, its width will tend

## first Voigt function



Fig. 6.9 Representation of $\Psi(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4}(x-y)^{2}}}{y^{2}+1} d y$
to increase, as predicted by the Doppler effect, which was described in its intuitive mode at the beginning of this chapter. In fact, due to self-shielding for an absorbing material, and given that $\sigma_{0}$ is not strictly constant, the area under the Voigt curve is weakly dependent on temperature. This dependence, which can be neglected for reactor physics applications, should not be forgotten in astrophysics, where the temperatures reached in the cores of stars are of the order of millions of Kelvin. A similar calculation shows that the resonance integral at infinite dilution $I_{\infty}$ is constant:

$$
I_{\infty}=\int_{0}^{\infty} \sigma(E) \frac{d E}{E}=\frac{\sigma_{0} \Gamma_{\gamma}}{\Gamma E_{0}} \int_{0}^{\infty} \frac{d E}{\left(\frac{E-E_{0}}{\Gamma / 2}\right)^{2}+1}
$$

Using the same reasoning as earlier, $d E / E$ is approximated by $d E / E_{0}$ since the contribution of neutrons with energy around is dominant in the integral term close to the resonance.

$$
\begin{aligned}
I_{\infty} & =\frac{\sigma_{0} \Gamma_{\gamma}}{\Gamma E_{0}} \int_{0}^{\infty} \frac{\frac{d E}{\Gamma / 2} \times \frac{\Gamma}{2}}{1+\left(\frac{E-E_{0}}{\Gamma / 2}\right)^{2}}=\frac{\sigma_{0} \Gamma_{\gamma}}{\Gamma E_{0}} \int_{\frac{-E_{0}}{T / 2}}^{+\infty} \frac{\frac{\Gamma}{2}}{1+x^{2}} d x \\
& =\frac{\sigma_{0} \Gamma_{\gamma}}{2 E_{0}} \int_{\frac{-E_{0}}{\Gamma / 2}}^{+\infty} \frac{1}{1+x^{2}} d x \approx \frac{\sigma_{0} \Gamma_{\gamma}}{2 E_{0}} \underbrace{\int_{-\infty}^{+\infty} \frac{1}{1+x^{2}} d x}_{\pi}
\end{aligned}
$$

Therefore, the resonance integral is equal to (Dresner 1960, p. 32):
Resonance integral of a sole capture resonance: $\quad I_{\infty}=\frac{\sigma_{0} \pi \cdot \Gamma_{\gamma}}{2 E_{0}}$

### 6.4.3 Interference Function

For the specific case of scattering, there is an interference term in the Breit-Wigner formalism, which is of the following form:

$$
\sigma_{s}(E)=\sqrt{\sigma_{s}(E) \sigma_{p} g} \frac{\Gamma_{n}}{\Gamma} \frac{2 x}{1+x^{2}}=\sigma_{t 0} \frac{R}{\lambda} \frac{\Gamma_{n}}{\Gamma} \frac{2 x}{1+x^{2}}
$$

with:

$$
\sigma_{p}=4 \pi R^{2}, \sigma_{t 0}(E)=4 \pi \lambda^{2} g \frac{\Gamma_{n}(E)}{\Gamma} \text { and } \sigma_{s 0}(E)=\sigma_{t 0}(E) \frac{\Gamma_{n}}{\Gamma}=4 \pi \lambda^{2} g \frac{\Gamma_{n}^{2}}{\Gamma^{2}}
$$

A calculation very similar to that for the first Voigt function leads to:

$$
\bar{\sigma}_{\text {interference }}=\sigma_{0} \frac{R \Gamma_{n}}{\lambda \Gamma} \chi(x, \xi)=\sigma_{0} \frac{R \Gamma_{n}}{\lambda \Gamma}\left[\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2 y}{y^{2}+1} e^{-\frac{\xi^{2}}{4}(x-y)^{2}} d y\right]
$$

The second Voigt function (also called the interference function) is defined by:

$$
\begin{equation*}
\text { Second Voigt function: } \quad \chi(x, \xi) \equiv \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2 y}{y^{2}+1} e^{-\frac{\xi^{2}}{4}(x-y)^{2}} d y \tag{6.11}
\end{equation*}
$$

Using the same logic as for the $\psi$ function, at low temperatures, the following is obtained:

$$
\bar{\sigma}(x)_{T \rightarrow 0 K}=\sigma_{0} \frac{R \Gamma_{n}}{\lambda_{0} \Gamma} \frac{2 x}{1+x^{2}}
$$

which is the interference term of the Breit-Wigner model. At high temperatures, similar to $\psi$, the exponential term can be assumed constant when $\xi$, which is inversely proportional to $\sqrt{T}$, is close to 0 . Hence, it can be taken out of the integral in $y$ by setting $y=0$. It can be seen that $2 y /\left(y^{2}+1\right)$ is an even function in $y$ and hence, its integral from $-\infty$ to $+\infty$ is equal to zero for all values of $x$. Hence, $\chi$ tends to the zero function at high temperatures and the interferences disappear. The function $\chi(x)$ is odd and has two symmetrical extrema (Fig. 6.10).

### 6.5 Application to the Large Resonance of Uranium 238

Let us consider the resonance situated at $E_{0}=6.64 \mathrm{eV}$ in the center-of-mass frame. This is a very important resonance for water reactors as it contributes significantly to resonant absorption.

Using $\Gamma=0.0265 \mathrm{eV}, \Gamma_{\gamma}=0.025 \mathrm{eV}, \sigma_{t 0}=21956$ barns

$$
\xi=\frac{\Gamma}{2} \sqrt{\frac{M}{\mu E_{0} k T}}=\frac{0.02651 .6 \cdot 10^{-19}}{2} \sqrt{\frac{238}{\frac{238 \times 1}{238+1} 6.641 .6 \cdot 10^{-19} 1.38 \cdot 10^{-23} T}} \approx \frac{8.56}{\sqrt{T}}
$$

Thus
$\sigma_{(n, \gamma)}(\xi, x)=\frac{\sigma_{t} \cdot \Gamma_{Y}}{\Gamma} \Psi(\xi, x)=21956 \quad \frac{0.025}{0.0265} \Psi(\xi, x)=20713.2 \Psi(\xi, x)_{[b a r n]}$
The radius of the nucleus is given approximately by the empirical formula (Evans 1955):

## Voigt's Interference Term



Fig. 6.10 Representation of the second Voigt function $\chi(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2 y}{y^{2}+1} e^{-\frac{\xi^{2}}{4}(x-y)^{2}} d y$

$$
R \approx 1.310^{-15} A^{1 / 3}=1.310^{-15} 238^{1 / 3}=8.05610^{-15} m
$$

The reduced wavelength is expressed in terms of the Planck constant, the neutron mass and the energy of the resonance:

$$
\lambda=\frac{h}{\pi \sqrt{8 m E_{0}}}=\frac{6.6210^{-34}}{3.14 \sqrt{81.6710^{-27} 6.641 .610^{-19}}}=1.76810^{-12} \mathrm{~m}
$$

Hence:

$$
\begin{aligned}
\sigma_{t}(x, T) & =\sigma_{t 0} \Psi(\xi, x)+\frac{\sigma_{t 0} R}{\lambda} \chi(\xi, x)+4 \pi R^{2} \\
& \left.=21956 \Psi(\xi, x)+100 \chi(\xi, x)+8.156_{[\text {barn }]}\right]
\end{aligned}
$$

The plot in Fig. 6.11 shows that the interference term decreases the cross section for $E<E_{0}$, and increases it for $E>E_{0}$. Furthermore, it can be noted that the higher the temperature, the lower is the interference term. Its impact is zero at the position of the resonance, although it modifies the wings of the latter: the left wing (before the resonance) is narrowed, while the right wing (after the resonance) is widened.

Total cross section of U238 with interference around the resonance at 6.64 eV


Fig. 6.11 Total cross section of ${ }_{92}^{238} U$
Nevertheless, this interference effect is quite weak for this particular resonance. The calculation of resonant absorption for the uranium 238 isotope must be carried out with extreme precision for PWR. On the other hand, $H T R$ with thorium are greatly impacted by the resonances of thorium 232, which is a fertile isotope with a large initial resonance at $21.8 \mathrm{eV} .{ }^{5}$

### 6.6 Temperature Effect on Cross Sections

Computing the Doppler feedback on a cross section eventually leads to the calculation of the derivatives of the Voigt functions with respect to temperature. Similarly, sensitivity analyses, which are usually carried out using perturbation models, use the analytical calculation of the Doppler effect, which is simpler than an experimental design method or using tabulated values. In a future chapter, we will return to the global effect of temperature on the reactivity of realistic fuel.

[^104]
### 6.6.1 First Voigt Function $\Psi$

We wish to calculate the derivative $\frac{\partial \Psi}{\partial T}(x, T)$ :

$$
\Psi(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}}}{1+y^{2}} d y \quad \text { and } \quad \xi=\frac{\Gamma}{\sqrt{\frac{4 \pi k T}{M}}}=\xi_{0} \sqrt{\frac{T_{0}}{T}}
$$

by defining the reference value of $\xi_{0}$ at $T_{0}: \xi_{0}=\Gamma / \sqrt{\frac{4 \pi \cdot k T_{0}}{M}}$.
Using the chain rule: $\frac{\partial \Psi}{\partial T}(x, T)=\frac{\partial \Psi}{\partial \xi} \frac{\partial \xi}{\partial T}(x, T)$ with $\frac{\partial \xi}{\partial T}(T)=-\frac{\xi_{0}}{2} \frac{\sqrt{T_{0}}}{T^{\frac{3}{2}}}=-\frac{\xi}{2 T}$
The term $\frac{\partial \Psi}{\partial \xi}$ is the derivative of the product of $\frac{\xi}{2 \sqrt{\pi}}$ and $f(x, \xi)=\int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4}(x-y)^{2}}}{1+y^{2}} d y$, i.e.:

$$
\frac{\partial \Psi}{\partial \xi}(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \frac{\partial f}{\partial \xi}(x, \xi)+\frac{1}{2 \sqrt{\pi}} f(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \frac{\partial f}{\partial \xi}(x, \xi)+\frac{\Psi(x, \xi)}{\xi}
$$

Only the derivative of $f(x, \xi)$ is now required. To calculate it, we use the theorem that allows differentiation under the integral sign, which states that if the function and its derivative can be integrated, then $\frac{\partial}{\partial x} \int f(x, t) d t=\int \frac{\partial f(x, t)}{\partial x} d t$.

So:

$$
\frac{\partial}{\partial \xi}\left(e^{-\frac{(x-y)^{2}}{4} \xi^{2}}\right)=-x^{2 \frac{\xi}{2}} e^{-\frac{(x-y)^{2}}{4} \xi^{2}}-\frac{\xi}{2} y^{2} e^{-\frac{(x-y)^{2}}{4} \xi^{2}}+x \frac{\xi}{2} 2 y \cdot e^{-\frac{(x-y)^{2}}{4} \xi^{2}}
$$

i.e.:
$\frac{\partial f}{\partial \xi}(x, \xi)=-x^{2} \frac{\xi}{2} \int_{-\infty}^{+\infty} \frac{e^{-\frac{(x-y)^{2}}{4} \xi^{2}}}{1+y^{2}} d y-\frac{\xi}{2} \int_{-\infty}^{+\infty} \frac{y^{2}}{1+y^{2}} e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y+x \frac{\xi}{2} \int_{-\infty}^{+\infty} \frac{2 y}{1+y^{2}} e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y$
In this expression, we find the functions $\sqrt{\pi} \Psi$ and $\sqrt{\pi} \chi=\frac{\xi}{2} \int_{-\infty}^{+\infty} \frac{2 y}{1+y^{2}} e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y$, therefore:

$$
\frac{\partial f}{\partial \xi}(x, \xi)=-x^{2} \sqrt{\pi} \Psi(x, \xi)-\frac{\xi}{2} \int_{-\infty}^{+\infty} \frac{y^{2}}{1+y^{2}} \cdot e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y+x \sqrt{\pi} \chi(x, \xi)
$$

Only the integral term in the middle remains. We find that $y^{2}=\left(y^{2}+1\right)-1$, which separates the integral into two parts:

$$
\frac{\xi}{2} \int_{-\infty}^{+\infty} \frac{y^{2}}{1+y^{2}} e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y=\frac{\xi}{2} \frac{2 \cdot \sqrt{\pi}}{\xi}-\sqrt{\pi} \Psi(x, \xi)
$$

thus: $\frac{\partial f}{\partial \xi}(x, \xi)=\sqrt{\pi}\left(1-x^{2}\right) \Psi(x, \xi)-\sqrt{\pi}+x \sqrt{\pi} \chi(x, \xi)$

Finally, in the final steps, the Voigt functions are themselves found in the derivative:

$$
\frac{\partial \Psi}{\partial \xi}(x, \xi)=\frac{\xi}{2}\left[\left(1-x^{2}+\frac{2}{\xi^{2}}\right) \Psi(x, \xi)-1+x \chi(x, \xi)\right]
$$

With the temperature variable, the following expression is obtained:
Temperature feedback on the first Voigt function:

$$
\begin{equation*}
\frac{\partial \Psi}{\partial T}(x, T)=-\frac{\xi^{2}}{4 T}\left[\left(1-x^{2}+\frac{2}{\xi^{2}}\right) \Psi(x, \xi)-1+x \chi(x, \xi)\right] \tag{6.12}
\end{equation*}
$$

### 6.6.2 Interference Function

The same procedure is applied to the interference function:

$$
\frac{\partial \chi}{\partial T}(x, T)=\frac{\partial \chi}{\partial \xi} \frac{\partial \xi}{\partial T}(x, T) \quad \text { with } \quad \frac{\partial \xi}{\partial T}(T)=-\frac{\xi_{0}}{2} \frac{\sqrt{T_{0}}}{T^{\frac{3}{2}}}=-\frac{\xi}{2 T}
$$

By setting $g(x, \xi)=\int_{-\infty}^{+\infty} 2 y \frac{e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}}}{1+y^{2}} d y$, we get the following:

$$
\frac{\partial \chi}{\partial \xi}(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \frac{\partial g}{\partial \xi}(x, \xi)+\frac{1}{2 \sqrt{\pi}} g(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \frac{\partial g}{\partial \xi}(x, \xi)+\frac{\chi(x, \xi)}{\xi}
$$

After some mathematical transformations:

$$
\begin{aligned}
\frac{\partial g}{\partial \xi}(x, \xi)= & -x^{2} \sqrt{\pi} \chi(x, \xi)-\frac{\xi}{2} \int_{-\infty}^{+\infty} 2 y \cdot e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y+\sqrt{\pi} \chi(x, \xi) \\
& +4 x \underbrace{\frac{\xi}{2}}_{2} \underbrace{\int_{-\infty}^{+\infty} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y}_{\frac{2}{\xi} \sqrt{\pi}}-4 x \sqrt{\pi} \psi(x, \xi)
\end{aligned}
$$

The term $\frac{\xi}{2} \int_{-\infty}^{+\infty} 2 y e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y$ can be computed by noticing that:

$$
2 y e^{-\frac{(x-y)^{2}}{4} \xi^{2}}=2 x e^{-\frac{(x-y)^{2}}{4} \xi^{2}}-\frac{4}{\xi^{2}} \frac{d\left(e^{-\frac{(x-y)^{2} \xi^{2}}{4} \xi^{2}}\right)}{d y}
$$

Thus: $\frac{\xi}{2} \int_{-\infty}^{+\infty} 2 y e^{-\frac{(x-y)^{2}}{4} \xi^{2}} d y=2 x x^{\frac{\xi}{2}} \underbrace{\int_{-\infty}^{+\infty} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y}_{\frac{2}{\xi} \sqrt{\pi}}-\underbrace{\frac{2}{\xi}}_{0}\left[e^{-\frac{(x-y)^{2}}{4} \xi^{2}}\right]_{-\infty}^{+\infty}=2 x \sqrt{\pi}$
Finally:

$$
\frac{\partial g}{\partial \xi}(x, \xi)=\sqrt{\pi}\left(2 x-x^{2} \chi(x, \xi)+\chi(x, \xi)-4 x \psi(x, \xi)\right)
$$

and:

Temperature feedback on the second Voigt function:

$$
\begin{equation*}
\frac{\partial \chi}{\partial T}(x, \xi)=-\frac{\xi}{2 T}\left[\xi x+\left(\frac{\xi}{2}\left(1-x^{2}\right)+\frac{1}{\xi}\right) \chi(x, \xi)-2 \xi x \psi(x, \xi)\right] \tag{6.13}
\end{equation*}
$$

For $x=0: \partial \chi(0, \xi) / \partial T=0$, which is consistent with the fact that the interference term is zero for any temperature (hence, for any value of $\xi$ ). For $x=0$, $T \frac{\partial \Psi}{\partial T}(0, \xi)=-\frac{\xi^{2}}{4}\left(\left(1+\frac{2}{\xi^{2}}\right) \Psi(0, \xi)-1\right)$. This coefficient is always negative as shown in Table 6.1. Therefore, for any temperature, the Voigt function is a decreasing function with temperature, and this phenomenon is exacerbated if the temperature rises. The result is the same for the second Voigt function.

### 6.6.3 Asymptotic Numeric Evaluation

Let the complex number $z$ be defined as $z=\xi(x+i) / 2$; the Voigt functions can be written as functions of integral of the complex probability density $W(z)$ :

$$
\psi(x, \xi)+i \chi(x, \xi)=\frac{\sqrt{\pi}}{2} \xi W(z)
$$

with: $W(z)=e^{-z^{2}} \operatorname{erfc}(-i z)=e^{z^{2}}\left(1+\frac{2 i}{\sqrt{\pi}} \int_{0}^{+\infty} e^{-y^{2}} d y\right)=\frac{1}{i \pi} \int_{-\infty}^{+\infty} \frac{e^{-y^{2}}}{y-z} d y$
For large values of $|z|>6$ (outside those of Tables 6.2 and 6.3), the following approximation can be used:
Table 6.1 Tabulation of the first Voigt function (Marguet, computed in 2009; using a Monte Carlo calculation ( $2.10^{6}$ trials) of the integral between -200 and +200 , standard deviation $<0.025 \%$ )
First Voigt function $\Psi(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{\frac{\xi^{2}}{4}(x-y)^{2}}{y^{2}+1} d y$

| $\xi / x$ | 0 | 0.3 | 0.5 | 1 | 2 | 4 | 6 | 8 | 10 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0.05 | 0.04309 | 0.04309 | 0.04308 | 0.04306 | 0.04298 | 0.04267 | 0.04216 | 0.04145 | 0.04055 |
| 0.10 | 0.08384 | 0.08382 | 0.08379 | 0.08364 | 0.08305 | 0.08073 | 0.07700 | 0.07208 | 0.06623 |
| 0.15 | 0.12239 | 0.12235 | 0.12223 | 0.12176 | 0.11989 | 0.11268 | 0.10165 | 0.08805 | 0.07328 |
| 0.20 | 0.15889 | 0.15868 | 0.15854 | 0.15748 | 0.15331 | 0.13777 | 0.11540 | 0.09027 | 0.06614 |
| 0.25 | 0.19347 | 0.19331 | 0.19281 | 0.19086 | 0.18324 | 0.15584 | 0.0071934 | 0.08277 | 0.05233 |
| 0.30 | 0.22624 | 0.22581 | 0.22516 | 0.22197 | 0.20968 | 0.16729 | 0.11571 | 0.07042 | 0.03880 |
| 0.35 | 0.25731 | 0.25650 | 0.25569 | 0.25091 | 0.23271 | 0.17288 | 0.00314 |  |  |
| 0.40 | 0.28679 | 0.28605 | 0.28450 | 0.27776 | 0.25245 | 0.17359 | 0.09604 | 0.0456 |  |
| 0.45 | 0.31477 | 0.31356 | 0.31168 | 0.30261 | 0.26909 | 0.17502 | 0.08439 | 0.03670 | 0.024 |
| 0.50 | 0.34135 | 0.33975 | 0.33733 | 0.32557 | 0.28286 | 0.16469 | 0.07346 | 0.03025 | 0.01446 |
| $\infty$ | 1.00000 | 0.91743 | 0.80000 | 0.50000 | 0.20000 | 0.05882 | 0.02703 | 0.01538 | 0.00990 |

Table 6.2 Tabulation of the second Voigt function (Marguet, computed in 2009, using a Monte Carlo calculation ( $2.10^{6}$ trials) of the integral between -200 and +200 , standard deviation $<0.025 \%$ )

| Second Voigt function $\chi(x, \xi)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2 y}{y^{2}+1} e^{-\frac{\xi^{2}}{4}(x-y)^{2}} d y$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $\xi / x$ | 0 | 0.3 | 0.5 | 1 |
| 0.05 | 0.00000 | 0.00072 | 0.00120 | 0.0023 |
| 0.10 | 0.00000 | 0.00275 | 0.00458 | 0.0091 |
| 0.15 | 0.00000 | 0.00592 | 0.00986 | 0.0196 |
| 0.20 | 0.00000 | 0.01009 | 0.01680 | 0.033 |
| 0.25 | 0.00000 | 0.01511 | 0.02515 | 0.049 |
| 0.30 | 0.00000 | 0.02087 | 0.03470 | 0.0687 |
| 0.35 | 0.00000 | 0.02725 | 0.04529 | 0.08 |
| 0.40 | 0.00000 | 0.03416 | 0.05674 | 0.1116 |
| 0.45 | 0.00000 | 0.04151 | 0.06890 | 0.1349 |
| 0.50 | 0.00000 | 0.04927 | 0.08165 | 0.1592 |
| $\infty$ | 0.00000 | 0.55046 | 0.80000 | 1.0000 |

Table 6.3 Decrease in the peak value of the effective cross section by Doppler effect

| $\xi$ | 0.05 | 0.10 | 0.15 | 0.20 | 0.25 | 0.30 | 0.35 | 0.40 | 0.45 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $-T \frac{\partial \Psi}{\partial T}(0, T)$ | 0.0209 | 0.0396 | 0.0563 | 0.0710 | 0.0841 | 0.0957 | 0.1059 | 0.1149 | 0.1227 |

$$
W(z)=\frac{i}{\sqrt{\pi}}\left[\alpha_{1} \frac{|z|^{2} \bar{z}-3 \alpha_{2} z}{|z|^{4}-6 \alpha_{2} \operatorname{Re}\left(z^{2}\right)+9 \alpha_{2}^{2}}+\alpha_{2} \frac{|z|^{2} \bar{z}-3 \alpha_{1} z}{|z|^{4}-6 \alpha_{1} \operatorname{Re}\left(z^{2}\right)+9 \alpha_{1}^{2}}\right]
$$

with $\alpha_{1}=\frac{1+\sqrt{\frac{2}{3}}}{2}$ and $\alpha_{2}=\frac{1-\sqrt{\frac{\sqrt{2}}{3}}}{2}$.

### 6.6.4 Derivatives of the Voigt Functions with Respect to Energy

The derivatives of the Voigt functions with respect to energy, via the reduced energy variable $x$, can also be useful in certain applications:

$$
\begin{aligned}
& \frac{\partial \Psi(x, \xi)}{\partial x}= \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{\partial}{\partial x}\left(\frac{e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}}}{1+y^{2}}\right) d y=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty}-\frac{\xi^{2}}{2}(x-y) \frac{e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}}}{1+y^{2}} d y \\
& \frac{\partial \Psi(x, \xi)}{\partial x}= \frac{\xi^{2}}{4} \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} 2 y \frac{e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}}}{1+y^{2}} d y-\frac{\xi^{2}}{2} x \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}}}{1+y^{2}} d y \\
& \quad=\frac{\xi^{2}}{2}\left(\frac{1}{2} \chi(x, \xi)-x \psi(x, \xi)\right)
\end{aligned}
$$

Similarly: $\frac{\partial x(x, \xi)}{\partial x}=\frac{\xi^{2}}{2} \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2 y^{2}}{y^{2}+1} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y-\frac{\xi^{2}}{2} x \chi(x, \xi)$
By noting that:

$$
\begin{aligned}
& \frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2 y^{2}}{y^{2}+1} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2\left(y^{2}+1\right)-2}{y^{2}+1} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y \\
& =\frac{\xi}{\sqrt{\pi}} \underbrace{\int_{-\infty}^{+\infty} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y}_{\frac{2}{\xi} \sqrt{\pi}}-\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{2}{y^{2}+1} e^{-\frac{\xi^{2}}{4} \cdot(x-y)^{2}} d y=2-2 \Psi(x, \xi)
\end{aligned}
$$

The following equation can be written:

$$
\frac{\partial \chi(x, \xi)}{\partial x}=\frac{\xi^{2}}{2}(2-2 \Psi(x, \xi))-\frac{\xi^{2}}{2} x \chi(x, \xi)=\xi^{2}\left(1-\Psi(x, \xi)-\frac{x}{2} \chi(x, \xi)\right)
$$

To sum up, the derivatives with respect to reduced energy are given by:

Derivatives of the Voigt functions with respect to energy:

$$
\left\{\begin{align*}
\frac{\partial \Psi(x, \xi)}{\partial x} & =\frac{\xi^{2}}{2}\left(\frac{1}{2} \chi(x, \xi)-x \psi(x, \xi)\right)  \tag{6.14}\\
\frac{\partial \chi(x, \xi)}{\partial x} & =\xi^{2}\left(1-\Psi(x, \xi)-\frac{x}{2} \chi(x, \xi)\right)
\end{align*}\right.
$$

In days when computers were less powerful, this system of coupled first-order differential equations allowed the calculation of the Voigt functions with analog circuits for a given temperature, i.e. with an imposed $\xi$. Historically, the functions $\psi$ and $\chi$ were studied under the following forms:

$$
\Psi(x, \beta)=\frac{1}{\beta \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{(x-y)^{2}}{\beta^{2}}}}{1+y^{2}} d y \quad \text { and } \quad \mathrm{X}(x, \beta)=\frac{1}{\beta \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{y}{1+y^{2}} e^{-\frac{(x-y)^{2}}{\beta^{2}}} d y
$$

with the same definition of $x=\left(E-E_{0}\right) / 2$ but $\beta=2 \Delta / \Gamma=2 / \xi$. Another difference is the coefficient value of 2 under the integral sign, which disappears when changing from $\chi(x, \xi)$ to $\mathrm{X}(x, \beta)$ since $\mathrm{X}(x, \beta)=\chi(x, \xi) / 2$. The Voigt functions will be denoted as $\Psi(x, \beta)$ and $X(x, \beta)$, or "Voigt profiles" (Dresner 1960, p. 35), to distinguish between these different functions.

### 6.6.5 Some Mathematical Properties of Voigt Profiles

These profiles are well suited to calculating the Doppler effect analytically. Their value at $x=0$ is given by:

$$
\left\{\begin{array}{c}
\Psi(0, \beta)=\frac{\sqrt{\pi}}{\beta} e^{\frac{1}{\beta^{2}}} \operatorname{erfc}\left(\frac{1}{\beta}\right) \\
X(0, \beta)=0
\end{array}\right.
$$

Similarly, for a temperature of zero:

$$
\left\{\begin{aligned}
\Psi(x, 0) & =\frac{1}{1+x^{2}} \\
\mathrm{X}(x, 0) & =\frac{x}{1+x^{2}}
\end{aligned}\right.
$$

The first profile is even, just like the first Voigt function. Similarly, the second profile is odd. The Voigt profiles can be expanded in converging series:

Series expansion of the Voigt profiles:

$$
\left\{\begin{align*}
\Psi(x, \beta) & =\frac{1}{\beta} e^{\frac{\left(1-x^{2}\right)}{\beta^{2}}} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{x}{\beta^{2}}\right)^{2 n} \Gamma\left(-n+\frac{1}{2}, \frac{1}{\beta^{2}}\right)  \tag{6.15}\\
\mathrm{X}(x, \beta) & =\frac{1}{\beta} e^{\frac{\left(1-x^{2}\right)}{\beta^{2}}} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{x}{\beta^{2}}\right)^{2 n+1} \Gamma\left(-n-\frac{1}{2}, \frac{1}{\beta^{2}}\right)
\end{align*}\right.
$$

where $\Gamma(a, t)$ is the incomplete gamma function defined by:

$$
\Gamma(a+1, t)=a \Gamma(a, t)+e^{t} t^{a}=\int_{t}^{\infty} x^{a} e^{-x} d x \quad \text { and } \quad \Gamma\left(\frac{1}{2}, t\right)=\sqrt{\pi} \operatorname{erfc}(\sqrt{t})
$$

The properties of the integral and derivatives of the Voigt profiles are given below:

$$
\left\{\begin{array} { l } 
{ \int _ { - \infty } ^ { + \infty } \Psi ( x , \beta ) d x = \pi } \\
{ \int _ { - \infty } ^ { + \infty } \mathrm { X } ( x , \beta ) d x = 0 }
\end{array} \text { and } \quad \left\{\begin{array}{l}
\frac{\partial \Psi(x, \beta)}{\partial x}=\frac{2}{\beta^{2}}(\mathrm{X}(x, \beta)-\Psi(x, \beta)) \\
\frac{\partial \mathrm{X}(x, \beta)}{\partial x}=\frac{2}{\beta^{2}}(1-\Psi(x, \beta)-\mathrm{X}(x, \beta))
\end{array}\right.\right.
$$

The differential equations obtained previously can be found for the Voigt functions using the transforms $\Psi(x, \beta)=\Psi(x, \xi)$ and $\mathrm{X}(x, \beta)=\chi(x, \xi) / 2$.

### 6.7 Effective Resonance Integral

### 6.7.1 Homogeneous Medium

Calculation of the effective resonance integral, especially that of uranium 238, is important for evaluating the escape factor (Duderstadt and Hamilton 1976, p. 334). For a homogeneous medium of resonant nuclei (uranium) and scattering nuclei (hydrogen and oxygen), the resonance integral for one situated at energy $E_{0}$, with the $N R$ approximation, is written as follows (using the equations obtained from the previous chapter):

$$
I_{0}=\int \sigma_{a}(u) \frac{\sigma_{p}}{\sigma_{t}(u)} d u
$$

The self-shielding coefficient $\sigma_{p} / \sigma_{t}(u)$ uses the potential scattering cross section, which is the sum of these cross sections for the resonant nuclei (uranium) and for the scattering nuclei of the mixture, normalized to one uranium atom: this cross section is sometimes called the dilution cross section $\sigma_{M}$. Since the medium is
homogeneous, the scattering cross section $\Sigma_{M}$ contains contributions from both the moderator and light nuclei of the fuel (e.g. oxygen in $\mathrm{UO}_{2}$ ):

$$
\sigma_{p}=\sigma_{p}^{U}+\frac{\Sigma_{M}}{N_{U}}=\sigma_{p}^{U}+\sigma_{M}
$$

Introducing the Doppler-broadened total cross section into the integral gives:

$$
\left\{\begin{array}{l}
\sigma_{t}(x)=\sigma_{p}+\sigma_{t 0} \psi(x, \xi)+\sqrt{\sigma_{t 0} \sigma_{p} g} \sqrt{\frac{\Gamma_{n}}{\Gamma}} \chi(x, \xi) \\
\sigma_{a}(x)=\sigma_{t 0} \frac{\Gamma_{a}}{\Gamma} \psi(x, \xi)=\sigma_{t 0} \frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{\Gamma} \psi(x, \xi)
\end{array}\right.
$$

with the usual notations ${ }^{6}$ :

$$
\beta \equiv \frac{\sigma_{p}}{\sigma_{t 0}}=\frac{\sigma_{p}^{U}+\sigma_{m}}{\sigma_{t 0}} \quad \text { and } \quad \zeta \equiv \frac{\sigma_{p}^{U}}{\sigma_{p}} \frac{\Gamma_{n}}{\Gamma}
$$

the following equation is obtained since $d u=\frac{\Gamma}{2 E_{0}} d x$ :

$$
I_{0}=\frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{2 E_{0}} \sigma_{p}\left[\int_{-\infty}^{+\infty} \frac{\psi(x, \xi)}{\psi(x, \xi)+\sqrt{\zeta \beta} \chi(x, \xi)+\beta} d x\right]
$$

For pins of small radii, the interference term is weak. In 1958, Adler, Hinmanand Nordheim tabulated the integral in the preceding formula. Let us set (Dresner 1960, p. 37; Duderstadt and Hamilton 1976, p. 336; Bussac and Reuss 1985, p. 127; Ferziger and Zweifel 1966, p. 109; Progress in nuclear energy Vol 2, 1958, p. 235):

$$
J(\xi, \beta)=\int_{0}^{+\infty} \frac{\psi(x, \xi)}{\psi(x, \xi)+\beta} d x
$$

so as to be able to write the effective resonance integral as:

$$
I_{0} \approx \frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{E_{0}} \sigma_{p} J(\xi, \beta)=\frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{E_{0}} \sigma_{t 0} \beta J(\xi, \beta)
$$

The function $J(\xi, \beta)$ was initially studied by Dancoff and Ginsburg in 1944. It was calculated precisely by Lawrence Dresner in 1956 (Dresner 1960, p. 37) and since then it has borne his name. For calculation codes, Keshavamurhty and Harish

[^105]proposed ${ }^{7}$ the use of the Pade approximation to perform the pseudo-analytical calculation quickly and accurately. It uses the first Voigt function. When the temperature tends to $0 K(\xi \rightarrow+\infty)$, the behavior of $\psi(x, \xi)$ is well known since the Breit-Wigner formalism is obtained, with a $1 /\left(1+x^{2}\right)$ function. Thus, (Dresner 1960, p. 37):
\[

$$
\begin{aligned}
\lim _{T \rightarrow 0 K} J(\xi, \beta) & =J(\infty, \beta)=\int_{0}^{+\infty} \frac{1}{1+\beta+\beta x^{2}} d x=\left[\frac{1}{\sqrt{(1+\beta) \beta}} \operatorname{Arctg}\left(\frac{\sqrt{(1+\beta) \beta}}{1+\beta} x\right)\right]_{0}^{+\infty} \\
& =\frac{\pi}{2 \sqrt{(1+\beta) \beta}}
\end{aligned}
$$
\]

If the dilution cross section tends to infinity, e.g. by decreasing the concentration of resonant isotopes, then, $\beta \gg 1 \geq \psi(x, \xi)$ :

$$
\lim _{\sigma_{m} \rightarrow 0} J(\xi, \beta)=\int_{0}^{+\infty} \frac{\psi(x, \xi)}{\beta} d x=\frac{\pi}{2 \beta}
$$

This can be interpreted as follows: if $\beta \gg 1 \geq \psi(x, \xi)$, only the area under the curve $\psi(x, \xi)$ contributes significantly to the integral. Hence, the resonance integral at infinite dilution is:

$$
I_{0}^{\infty}=\frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{E_{0}} \sigma_{p} \frac{\pi}{2 \beta}=\frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{E_{0}} \sigma_{t 0} \frac{\pi}{2}
$$

Applying this equation only to capture, the result from Eq. (6.10) is obtained. The mathematical analysis of the function $J(\xi, \beta)$ shows that it decreases with $\xi$. This is due to the fact that a rise in temperature causes an increase in $J(\xi, \beta)$, and hence in the absorption integral. Indeed:

$$
\frac{\partial J(\xi, \beta)}{\partial \xi}=\beta \int_{0}^{+\infty} \frac{\frac{\partial \psi(x, \xi)}{\partial \xi}}{(\psi(x, \xi)+\beta)^{2}} d x
$$

Since $\frac{\partial^{2} \psi(x, \xi)}{\partial \xi^{2}}=-\frac{\xi^{3}}{2} \frac{\partial \psi(x, \xi)}{\partial \xi}$, using integration by parts:

[^106]\[

$$
\begin{aligned}
\frac{\partial J(\xi, \beta)}{\partial \xi}= & -\frac{2 \beta}{\xi^{3}} \int_{0}^{+\infty} \frac{\frac{\partial^{2} \psi(x, \xi)}{\partial \xi^{2}}}{(\psi(x, \xi)+\beta)^{2}} d x=-\frac{2 \beta}{\xi^{3}} \underbrace{\left[\frac{\frac{\partial \psi(x, \xi)}{\partial \xi}}{(\psi(x, \xi)+\beta)^{2}}\right]_{0}^{+\infty}}_{0} \\
& -\frac{4 \beta}{\xi^{3}} \int_{0}^{+\infty} \frac{\left(\frac{\partial \psi(x, \xi)}{\partial \xi}\right)^{2}}{(\psi(x, \xi)+\beta)^{3}} d x<0
\end{aligned}
$$
\]

Hence, the Dresner integral increases with temperature (Dresner 1960, p. 39). Substituting $\left(\Gamma_{\gamma}+\Gamma_{f}\right)$ by $\Gamma_{\gamma}$ immediately shows that the capture integral also increases. This is a very important result for reactor safety since it shows that the Doppler effect compensates inserted reactivity during power excursions because of the increase of the fuel temperature. Moreover, the Doppler effect is more efficient if the fuel is a poor heat conductor, as is the case with oxide fuel. In realistic cases where $\xi \sqrt{\pi} / 2 / \beta \gg 1$, then (Dresner 1960, 40):

$$
J(\xi, \beta) \approx \frac{2}{\xi} \sqrt{\ln \left(\frac{\sqrt{\pi}}{2} \frac{\xi}{\beta}\right)}
$$

Expansion into converging series ${ }^{8}$ allows precise calculation of the Dresner integral for other situations:

$$
J(\xi, \beta)=\frac{\pi}{2 \beta} \sum_{n=0}^{\infty} B_{n} u^{n} \quad \text { with }: \quad u \equiv \frac{v}{1+v}, \quad v \equiv \frac{\sqrt{\pi}}{2 \beta} \xi e^{\frac{\xi^{2}}{4}} \operatorname{erfc}\left(\frac{\xi}{2}\right)
$$

And $B_{n} \equiv\left\{\begin{array}{l}A_{0} \\ \sum_{m=1}^{n} C_{m-1}^{n-1} A_{m} \quad m \geq 1\end{array}\right.$ with: $A_{m} \equiv \frac{(-1)^{m}}{\sqrt{1+m}}$ (Fig. 6.12, Photo 6.3).

### 6.7.2 Heterogeneous Medium

(Ferziger and Zweifel 1966, p. 110)
In the 1950s, the influence of the heterogeneous nature of the medium on the effective resonance integral was rapidly observed. Empirical formulae were largely

[^107]Fig. 6.12 Dresner function (from Dresner 1960, p. 43)

Photo 6.3 Lawrence
Dresner (Courtesy Dresner)


set up (Lamarsh and Barrata 2001, p. 371; Bussac and Reuss 1985, p. 308; Progress in Nuclear Energy, Vol 2, 1958, pp. 249-250):

$$
I_{[b a r n]}=a+\frac{b}{\sqrt{\rho_{\left[\mathrm{g} / \mathrm{cm}^{3}\right]} R_{[\mathrm{cm}]}}} \quad \text { or } \quad I_{[b a r n]}=c+d \sqrt{\frac{S_{\left[\mathrm{cm}{ }^{2}\right]}}{M_{[\mathrm{g}]}}}
$$

where $R$ is the radius of the fuel pin, $\rho$ is its density and, $a$ and $b$ are constants which are fitted experimentally (for $U O_{2}, a=3, b=39.6, \rho=10.95 \mathrm{~g} / \mathrm{cm}^{3}$ ), or alternatively $S$ is the effective resonance surface, ${ }^{9}$ which coincides with the outer surface of the pin where the cell contains only one pin, and $M$ is its mass (for $U O_{2}, c=5.35$, $d=26.6$ ). In the meantime, the analytical calculation of $I_{\text {eff }}$ was being developed. In the case of a lattice of fuel pins in a moderator, among neutrons undergoing collisions in the fuel, those which undergo their final collision in the moderator are distinguished from those having their final collision in the fuel. Neutrons coming from water are characterized by the probability $P_{M c}$ since they come from the moderator $M$ outside the fuel pin to interact with the resonant isotope in the fuel (Fig. 6.13).

For the time being, it is assumed that the resonances are well separated and an asymptotic $1 / E$ flux shape may be used outside the resonances. Using the Narrow Resonance approximation, it is considered that any scattering collision removes the neutron from the resonance zone. To ensure that the $N R$ approximation is applicable, we shall compare the resonance width $\Gamma_{p}=\Gamma \sqrt{\sigma_{t 0} / \sigma_{p}}$ (i.e. the energy range where the cross section is twice the potential cross section) with the maximum energy loss per collision at the resonance energy, i.e. $E_{0}(1-\alpha)$. The neutron

Fig. 6.13 Definition of probabilities for the resonance integral


[^108]balance is obtained from the slowing-down equation of a non-leaking medium, written such that the usual slowing-down operators (with brackets) for the fuel $R_{c}[]$ and moderator $R_{M}[]$ are:
\[

$$
\begin{aligned}
V_{c} \Sigma_{t}^{c}(E) \Phi_{c}(E) & =V_{c} \underbrace{\left(1-P_{c M}\right)}_{P_{c c}} \int_{E}^{\frac{E}{\alpha_{c}}} \frac{\Sigma_{s}^{c}\left(E^{\prime}\right) \Phi_{c}\left(E^{\prime}\right)}{\left(1-\alpha_{c}\right) E^{\prime}}+V_{M} P_{M c} \int_{E}^{\frac{E}{\alpha_{M}}} \frac{\Sigma_{s}^{M}\left(E^{\prime}\right) \Phi_{M}\left(E^{\prime}\right)}{\left(1-\alpha_{M}\right) E^{\prime}} \\
& =V_{c}\left(1-P_{c M}\right) R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+V_{M} P_{M c} R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right]
\end{aligned}
$$
\]

The first term on the RHS is the contribution of neutrons scattering in the fuel, without emerging from it (with a probability $\left(1-P_{c M}\right)$ where $P_{c M}$ is the probability of leaking out of the fuel without any collision). In the same time, the second term represents the contribution of neutrons which scatter in the moderator and reach the fuel without undergoing any collision, with a probability of $P_{M C}$. The leakage probabilities are related to one another by the reciprocity theorem which will be studied in more detail in the chapter on the Boltzmann equation:

$$
V_{c} P_{c M} \Sigma_{t}^{c}=V_{M} P_{M c} \Sigma_{t}^{M} \approx V_{M} P_{M c} \Sigma_{s}^{M}
$$

Moreover, as we saw in the previous chapter on resonant absorption, in the $N R$ approximation, the moderator flux has a $1 / E$ shape when normalizing to an asymptotic flux. Hence, by assuming that the moderator scattering cross section $\Sigma_{s}^{M}$ depends weakly on energy, leading to a simplification of the slowing-down operator in the moderator, we obtain:

$$
R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right] \approx \frac{\Sigma_{s}^{M}}{E}
$$

Furthermore, it can also be assumed that only potential scattering contributes to neutron scattering in the fuel (by neglecting for the time being the fuel moderator $m$ scattering resonances in the pin and the scattering resonances of uranium). Thus:

$$
R_{c}\left[\Sigma_{s}^{c} \boldsymbol{\Phi}_{c}\right] \approx \frac{\Sigma_{p}^{c}}{E}
$$

Using these slowing-down operator simplifications and the reciprocity theorem, the flux in the fuel and in the moderator can be uncoupled in the balance equation:

$$
\begin{equation*}
\text { NR flux with two zones: } \quad \Phi_{c}^{N R}(E)=\frac{\left(1-P_{c M}\right) \Sigma_{p}^{c}+P_{c M} \Sigma_{t}^{c}}{E \Sigma_{t}^{c}(E)} \tag{6.16}
\end{equation*}
$$

If $P_{c M}$ can be computed, the flux can be computed analytically in the fuel. By writing the balance equation in the moderator, the flux in the latter is:

$$
V_{m} \Sigma_{t}^{m} \Phi_{m}(E)=V_{c} P_{c M} R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+V_{M}\left(1-P_{M c}\right) R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right]
$$

The effective absorption integral in lethargy for a resonance located at $E_{0}$ is then obtained as follows (given that $d u=d E / E)^{10}$ :

$$
\begin{aligned}
I_{0}^{N R} & =\int \sigma_{a}(u) \Phi_{c}^{N R}(u) d u=\int \sigma_{a}(u)\left[\left(1-P_{c M}\right) \frac{\sigma_{p}}{\sigma_{t}(u)}+P_{c M}\right] d u \\
& =\underbrace{\int \sigma_{a}(E) \frac{\sigma_{p}}{\sigma_{t}(u)} d u}_{\text {Volume integral }}+\underbrace{\int \sigma_{a}(u) \frac{\sigma_{t}(u)-\sigma_{p}}{\sigma_{t}(u)} P_{c M} d u}_{\text {Surface integral }}
\end{aligned}
$$

In this expression, the potential cross section is the sum of:

- the potential cross section of the heavy nucleus (uranium), hence without its resonant contribution,
- the fuel potential dilution cross section, not to be confused with the moderator dilution cross section, which is the potential cross section corresponding to non-resonant moderator nuclei in the fuel (oxygen in $\mathrm{UO}_{2}$ ), given for one uranium atom. The latter is calculated as:

$$
\sigma_{p}=\sigma_{p}^{U}+\frac{\Sigma_{p}^{m}}{N_{U}}
$$

$\sigma_{p}$ is assimilated to an equivalent (non-resonant) potential cross section for the fuel. The resonance integral is written in the form of a volume integral, which characterizes neutrons scattering from the fuel, and a surface integral, which takes into account the contribution of neutrons scattering from the moderator at the fuel surface (the reader should note that the integral is computed on the energy variable!). If a fuel pin is assumed to be independent of the other surrounding pins, the escape probability without scattering, $P_{c M}$, is computed by the formula on the chord length as will be seen in the chapter on the Boltzmann equation:

$$
P_{c M}=\frac{\int_{0}^{\infty} p(R)\left(1-e^{-N_{U} \sigma_{t} R}\right) d R}{N_{U} \sigma_{t}\langle R\rangle}
$$

where $\langle R\rangle=4 V / S$ is the mean chord length and (Cauchy theorem) and $p(R) d R$ is the probability of obtaining a chord of length $R$ up to $d R$. For coupled pins, the neutrons can come directly from a surrounding pin. This is called the shadowing effect or Dancoff effect, which complicates the integral. It will be computed later on in

[^109]Chap. 14. To simplify calculations, an escape cross section $\sigma_{e}$ is defined to express the escape probability without scattering in a rational form:

$$
P_{c M} \equiv \frac{\sigma_{e}}{\sigma_{e}+\sigma_{t}^{c}(E)} \quad \text { i.e. }: \quad \sigma_{e} \equiv \frac{P_{c M}}{1-P_{c M}} \sigma_{t}^{c}(E)
$$

This cross section depends weakly on energy. Using a constant leakage value in energy $\sigma_{e}=1 /\left(N_{U}\langle R\rangle\right)$, Eugen Wigner approximated the probability $P_{c M}$ as (Weinberg and Wigner 1958; Dresner 1960, p. 60):

$$
P_{c M}^{\text {Wigner }} \approx \frac{1}{1+N_{U}<R>\sigma_{t}}=\frac{1}{1+z \frac{\sigma_{t}}{\sigma_{p}}} \approx \frac{1}{1+z\left(\frac{\psi(x, \xi)}{\beta}+1\right)}
$$

by introducing the following notations:

$$
\beta \equiv \frac{\sigma_{p}}{\sigma_{t 0}}=\frac{\sigma_{p}^{U}+\frac{\Sigma_{m}}{N_{U}}}{\sigma_{t 0}} \equiv \frac{\sigma_{p}^{U}+\sigma_{m}}{\sigma_{t 0}}, \quad \tau \equiv \frac{\sigma_{p}^{U}}{\sigma_{p}} \frac{\Gamma_{n}}{\Gamma} \quad \text { and } \quad z \equiv N_{U} \sigma_{p}\langle R\rangle
$$

and by neglecting the interference function in the total cross section. The rational approximation is sufficient for most resonances. It can be noted that for $N_{U}<R>\sigma_{t} \gg 1, \quad P_{c M}^{\text {Wigner }} \propto 1 /\left(<R>\Sigma_{t}\right), \quad$ and $\quad$ for $\quad N_{U}<R>\sigma_{t} \ll 1$, $P_{c M}^{\text {Wigner }} \approx 1$, which is logical in the case of weakly absorbing media or very small media for example. This approximation can be bettered by introducing a constant value $n$ between 2 and 3, even if the limit of $n$ at infinity is around $n=3 / 4$ :

$$
P_{c M} \approx \frac{1}{1+N_{U}\langle R\rangle \sigma_{t}-\frac{N_{U}\langle R\rangle \sigma_{t}}{N_{U}\langle R\rangle \sigma_{t}+n}}
$$

A similar approach has been proposed by Carlvik in 1964 to compute the resonance integral (it will be described in Chap. 14 as it employs the concept of multicells). Using a similar mathematical formalism as for homogeneous calculations, the resonance integral is written as:

$$
I_{0}=\frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{2 E_{0}} \sigma_{p}\left[\begin{array}{l}
\int_{-\infty}^{+\infty} \frac{\psi(x, \xi)}{\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)+\beta} d x \\
+\int_{-\infty}^{+\infty} \psi(x, \xi) \frac{\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)}{\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)+\beta} P_{c M} d u
\end{array}\right]
$$

where $P_{c M}$ is a function of $\left(\frac{z}{\beta}(\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)+\beta)\right)$

The following functions are thus defined (Silvennoinen 1976, p. 167):

$$
\left\{\begin{aligned}
J(\xi, \beta) & =\int_{0}^{+\infty} \frac{\psi(x, \xi)}{\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)+\beta} d x \\
\alpha(\xi, \beta, z) & =\int_{0}^{+\infty} \psi(x, \xi) \frac{\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)}{\psi(x, \xi)+\sqrt{\tau \beta} \chi(x, \xi)+\beta} P_{c M}(x, \xi, z) d x
\end{aligned}\right.
$$

to simplify the expression of the absorption integral as follows (using the fact that all terms in the integrals are even, thus cancelling the two and integrating over $[0,+\infty[$ only):

$$
I_{0}=\frac{\left(\Gamma_{\gamma}+\Gamma_{f}\right)}{E_{0}} \sigma_{p}\left[J(\xi, \beta)+\frac{1}{\beta} \alpha(\xi, \beta, z)\right]
$$

When the interference function is neglected, the function simplifies to $L(\xi, \beta, z)=\int_{0}^{+\infty} \frac{\psi^{2}(x, \xi)}{\psi(x, \xi)+\beta} P_{c M}(x, \xi, z) d x$, which was calculated by Adler and Nordheim at the end of the 1950s for different geometries.

In the unresolved range, a statistical approach can be used to compute the contribution of the resonances to the effective absorption integral. Assuming that the scattering widths have a Porter-Thomas distribution ${ }^{11}$ (Foderaro 1971, p. 283) such that:

$$
\left\{\begin{array}{l}
\Gamma_{n}^{0}=y<\Gamma_{n}^{0}> \\
\Gamma_{n}=\Gamma_{n}^{0} \sqrt{E} \\
p(y) d y=\frac{1 e^{-\frac{y}{2}}}{\sqrt{2 \pi} \sqrt{y}} d y
\end{array}\right.
$$

The mean integral resonance in a range $d E$ with resonance spacing $D$ can be defined as:

$$
\overline{I(E)}=I(E) \frac{d E}{D}
$$

The contribution to the resonance integral above $E$ is written as:

[^110]$$
I(E)=\int_{E}^{+\infty} \sigma_{a}^{\text {effective }} \frac{d E^{\prime}}{E^{\prime}}=\frac{1}{D} \int_{E}^{+\infty} d E^{\prime} \int_{0}^{+\infty} I\left(E^{\prime}\right) p(y) d y
$$

If the $N R$ hypothesis is not acceptable for a resonance, e.g. for fuel with slowingdown nuclides, as in the case of oxygen in oxide fuel, a dilution factor $\sigma_{m}=\Sigma_{m} / N_{U}$ should be taken into account and the volume and surface integrals will consequently be modified:

$$
\left\{\begin{array}{l}
I_{v 0}=\int \sigma_{a}(u) \frac{\sigma_{m}}{\sigma_{a}(u)+\sigma_{m}} d u \\
I_{S 0}=\int \sigma_{a}(u) \frac{\sigma_{a}(u)}{\sigma_{a}(u)+\sigma_{m}} P d u
\end{array}\right.
$$

with: $P=\frac{P_{c h}\left(N_{U}\langle R\rangle \sigma_{t}\right)}{1-\left[1-\frac{\left.\sigma_{t+\sigma}+\sigma_{t}\right]}{\sigma_{t}}\right] P_{M_{c}}\left(N_{U}\langle R\rangle \sigma_{t}\right)}$

### 6.7.3 Analytical Calculation of a Broadened Resonance: The Campos-Martinez Model

The resonance integral for an isolated resonance can be derived analytically in heterogeneous geometries. In the previous chapter on resonant absorption, the Livolant-Jeanpierre model and its extension to a fuel pin surrounded by moderator was described. Using the Dresner functions, the approach for narrow resonances has been set up. Yet, it does not take into account any moderating nuclides in the fuel. Campos and Martinez ${ }^{12}$ worked out an approach based on the analytical calculation of $P_{c c}$ for a cylindrical geometry, which is precise enough for many applications. The same notations as for the resonant absorption description will be used here. Given a fuel pin containing a heavy resonant isotope (indexed $U$ ) combined with a light moderating isotope (indexed $m$ ), in a moderator channel (indexed M) (Fig. 6.14):

The neutron balance equations using the first-collision probabilities are:

$$
\left\{\begin{aligned}
& V_{c} \Sigma_{t}^{c} \Phi_{c}=V_{c}\left(1-P_{c M}\right) R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+V_{M} P_{M c} \\
& R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right] \\
& V_{M} \Sigma_{t}^{M} \Phi_{M}=V_{c} P_{c M} \\
& R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+V_{M}\left(1-P_{M c}\right) R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right]
\end{aligned}\right.
$$

[^111]Fig. 6.14 The geometry considered in the CamposMartinez model

where $R_{j}\left[\Sigma_{s} \Phi\right]=\int_{E}^{\frac{E}{\alpha_{j}}} \frac{\Sigma_{s} \Phi\left(E^{\prime}\right)}{\left(1-\alpha_{j}\right) E^{\prime}} d E^{\prime}$ is the operator for slowing-down by collision with an isotope characterized by $\alpha_{j}=\left(A_{j}-1\right)^{2} /\left(A_{j}+1\right)^{2}$. The cross sections are modeled using a Breit-Wigner formalism with Doppler broadening at temperature using the Voigt functions described previously:

$$
\left\{\begin{array}{l}
\sigma_{n, \gamma}(E)=\sigma_{0} \frac{\Gamma_{\gamma}}{\Gamma} \psi(x, \xi) \\
\sigma_{s}(E)=\sigma_{p}+\sigma_{0} \frac{\Gamma_{n}}{\Gamma} \psi(x, \xi)+\sqrt{\sigma_{0} \sigma_{p} \frac{\Gamma_{n}}{\Gamma}} \chi(x, \xi)
\end{array}\right.
$$

From now on, we will ignore the effect of the interference function $\chi(x, \xi)$ on the scattering cross section. The Campos-Martinez model does not use the Wigner rational approximation but rather a model for the escape probability from the rod $P_{c M}$, using an approximation based on the mean chord length $\langle\ell\rangle$ (obtained by expanding the non-interacting probability up to order three close to the mean chord):

$$
P_{c M}=\frac{1}{1+\Sigma_{t}^{c} \cdot\langle\ell\rangle}+A_{1} \frac{\Sigma_{t}^{c} \cdot\langle\ell\rangle}{\left(1+\Sigma_{t}^{c} \cdot\langle\ell\rangle\right)^{3}}+A_{2} \frac{\left.\left(\Sigma_{t}^{c} \cdot\langle \rangle\right\rangle\right)^{2}}{\left(1+\Sigma_{t}^{c} \cdot\langle\ell\rangle\right)^{4}}
$$

In this equation, the total cross section of the fuel is:

$$
\Sigma_{t}^{c}=\Sigma_{t}^{U}+\Sigma_{t}^{m} \approx N_{U}\left(\sigma_{n, \gamma}^{c}+\sigma_{s}^{c}+\frac{\Sigma_{s}^{m}}{N_{U}}\right) \equiv N_{U} \sigma_{t}^{c}
$$

which thus gives the definition for the microscopic cross section $\sigma_{t}^{c}$, brought to $N_{U}$, the number of resonant isotope nuclides. Henceforth, $\sigma_{m} \equiv \Sigma_{s}^{m} / N_{U}$ denotes the scattering cross section for the moderator mixed with heavy nuclides in the fuel, and brought to the amount of absorbing heavy nuclides (worth around 8 barns for
oxygen in uranium oxide). By substituting the equations for Doppler-broadened cross sections, a polynomial form is obtained for the escape probability:

$$
\left\{\begin{array}{lc}
P_{c M}=s+\left(A_{1}+A_{2}\right) s^{2}+\left(A_{1}+2 A_{2}\right) s^{3}+A_{2} s^{4} & s=\frac{\sigma_{g}}{\psi+\beta_{c}} \\
\beta_{c}=\frac{\sigma_{m}+\sigma_{p}^{U}}{\sigma_{0}+\sigma_{g}} & \sigma_{g}=\frac{\sigma_{e}}{\sigma_{0}} \\
\sigma_{e}=\frac{1}{N_{U} \cdot\langle\ell\rangle} & \sigma_{p}^{U}=\text { potential section of the resonant isotope }
\end{array}\right.
$$

The neutron balance equations are simplified using the reciprocity relations of $P_{i j}$ :

$$
P_{c M} V_{c} \Sigma_{t}^{c}=P_{M c} V_{M} \Sigma_{t}^{M}
$$

and by computing the slowing down term for the moderator in the fuel cell using the narrow resonance approximation. It is thus assumed that the flux has a $1 / E$ shape outside the resonance (this assumption is equivalent to normalizing the asymptotic flux which has a $C s t /\left(\overline{\xi \Sigma_{s}} E\right)$ shape Duderstadt and Hamilton 1976, p. 429):

$$
R_{M}\left[\Sigma_{s} \Phi\right]=\int_{E}^{\frac{E}{\alpha_{M}}} \frac{\sum_{s}^{M} \Phi\left(E^{\prime}\right)}{\left(1-\alpha_{M}\right) E^{\prime}} d E^{\prime} \approx \Sigma_{s}^{M} \int_{E}^{\frac{E}{\alpha_{M}}} \frac{1}{\left(1-\alpha_{M}\right) E^{\prime 2}} d E^{\prime}=\frac{\Sigma_{s}^{M}}{E}
$$

Hence:

$$
\begin{aligned}
V_{c} \Sigma_{t}^{c} \Phi_{c}= & V_{c}\left(1-P_{c M}\right) R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right] \\
& +V_{M} P_{M c} \frac{\Sigma_{s}^{M}}{E}=V_{c}\left(1-P_{c M}\right) R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+\frac{P_{c M} V_{c} \Sigma_{t}^{c}}{\Sigma_{t}^{M}} \frac{\Sigma_{s}^{M}}{E}
\end{aligned}
$$

The slowing-down kernel is developed into two terms. The first one is the slowing-down kernel for the resonant isotope, which can be modeled by the narrow resonance (NR), intermediate resonance (IR), or wide resonance (WR) approximation, according to the given resonance. The second term is that for the moderator for which the narrow resonance is a satisfactory approximation:

$$
R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]=R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+R_{m}\left[\Sigma_{s}^{m} \Phi_{c}\right]=\lambda \frac{\Sigma_{p}^{U}}{E}+(1-\lambda) \Sigma_{s}^{U} \Phi_{c}+\frac{\Sigma_{s}^{m}}{E}
$$

Here, the slowing-down kernel for a heavy nucleus is modeled by the interpolation between the $N R$ and $W R$ models using the intermediate resonance parameter $\lambda$. Introduced in 1962 by Rubin Goldstein and Cohen (Stamm'ler and Abbate 1983, p. 306; Silvennoinen 1976, p. 156; Reactor Physics 1966, p. 37), these parameters
play an important role. They are sensitive to temperature variations only for heavy nuclei and are difficult to evaluate. ${ }^{13}$ In particular, they can be negative or greater than 1 (!), a much unlikely fact given their definition. These simplifications allow the computation of the flux in the fuel:

$$
\Phi_{c}=\frac{\sigma_{m}+\lambda \sigma_{p}^{U}+P_{c M}\left(\sigma_{n, \gamma}^{U}+\lambda \sigma_{s, \text { Rés }}^{U}\right)+P_{c M}(1-\lambda) \sigma_{s}^{U}}{\sigma_{m}+\sigma_{n, \gamma}^{U}+\lambda \sigma_{s}^{U}+P_{c M}(1-\lambda) \sigma_{s}^{U}} \frac{1}{E}
$$

In this equation, in the denominator, the term $\mu=P_{c M}(1-\tau) \sigma_{s}^{U}$ is negligible compared to the resonant cross section $\sigma_{n, \gamma}^{U}$. In the numerator, only the term for the resonant scattering cross section is retained. Thus:

$$
\Phi_{c} \approx \frac{\sigma_{m}+\lambda \sigma_{p}^{U}+P_{c M}\left(\sigma_{n, \gamma}^{U}+\sigma_{s, \text { Rés }}^{U}\right)}{\sigma_{m}+\sigma_{n, \gamma}^{U}+\lambda \sigma_{s}^{U}} \frac{1}{E}
$$

In the wide resonance approximation, or even in the intermediate resonance model, the infinitely-heavy nucleus approximation results in assuming that a collision with a heavy nucleus leads to a very low energy loss such that the neutron remains within the resonance. The potential cross section of the heavy nucleus may thus be ignored using the term $P_{c M} \sigma_{p}^{U}$. Introducing the Voigt function, the following is found:

$$
\left\{\begin{array}{l}
\Phi_{c} \approx\left(\frac{\beta_{R}}{\psi+\beta_{R}}+(1+G(\lambda)) P_{c M} \frac{\psi}{\psi+\beta_{R}}\right) \frac{1}{E} \quad, \quad G(\lambda)=(1-\lambda) \frac{\Gamma_{n}}{\Gamma_{R}} \\
\beta_{R}=\frac{\sigma_{p}^{R}}{\sigma_{0}^{R}} \quad, \quad \sigma_{p}^{R}=\sigma_{m}+\lambda \sigma_{p}^{U} \quad, \quad \sigma_{0}^{R}=\sigma_{0} \frac{\Gamma_{R}}{\Gamma} \quad, \quad \Gamma_{R}=\Gamma_{\gamma}+\lambda \Gamma_{n}
\end{array}\right.
$$

Using this equation for flux in the fuel, the resonance integral is computed as:

$$
\begin{aligned}
I & =\int_{E_{0}} \sigma_{n, \gamma}(E) \Phi_{c}(E) d E=\int_{-\infty}^{+\infty} \sigma_{0} \Gamma_{\gamma} \Phi_{c} \frac{d E}{\Gamma} \\
& =\frac{\sigma_{0} \Gamma_{\gamma}}{E_{0}}\left[\beta_{R} \int_{0}^{\infty} \frac{\psi}{\psi+\beta_{R}} d x+(1+G(\lambda)) \int_{0}^{\infty} P_{c M} \frac{\psi^{2}}{\psi+\beta_{R}} d x\right]
\end{aligned}
$$

using $d x=2 d E / \Gamma$ and the fact that the functions in the integral sign are even (thereby, cancelling the 2 by integrating over $[0,+\infty]$ only), and by removing from the integral the dominant term in energy at resonance energy $E_{0}$. The leakage

[^112]probability $P_{C M}$ is substituted by its polynomial form, thereby introducing the Dresner function:
\[

$$
\begin{gathered}
J(\xi, \beta)=\int_{0}^{\infty} \frac{\psi(x, \xi)}{\psi(x, \xi)+\beta} d x \\
I= \\
\frac{\sigma_{0} \Gamma_{\gamma}}{E_{0}} \beta_{R} \int_{0}^{\infty} \frac{\psi}{\psi+\beta_{R}} d x+(1+G(\lambda)) \int_{0}^{\infty}\left[\frac{\sigma_{g}}{\psi+\beta_{c}}+\left(A_{1}+A_{2}\right)\left(\frac{\sigma_{g}}{\psi+\beta_{c}}\right)^{2}\right. \\
\\
\left.+\left(A_{1}+2 A_{2}\right)\left(\frac{\sigma_{g}}{\psi+\beta_{c}}\right)^{3}+A_{2}\left(\frac{\sigma_{g}}{\psi+\beta_{c}}\right)^{4}\right] \frac{\psi^{2}}{\psi+\beta_{R}} d x
\end{gathered}
$$
\]

The second integral term can be modified to introduce the successive derivatives of the Dresner function up to order 3. Besides, several analytical approximations to the Dresner function are available (the Steen formula ${ }^{14}$ for instance). The CamposMartinez model can then be employed to calculate the contribution of a resonance to the heterogeneous resonant absorption analytically (save for the evaluation of the Dresner function) with a precision of $2 \%$. The degree of freedom $\lambda$ is still the fraction which encompasses the intermediate character of the resonance. Campos and Martinez propose compares the practical resonance width (depending on the temperature, and such that the cross section is twice larger than the potential cross section) $\Gamma_{p}(T)$ to the energy loss per collision $\overline{\Delta E}$. For a narrow resonance $\overline{\Delta E} / \Gamma_{p}(T) \gg 1$, while for a wide resonance the converse is obtained, giving an exponential equation:

$$
\lambda=1-e^{-\kappa \frac{\bar{E}}{T_{p}(T)}}
$$

$\kappa$ is an empirical parameter which depends on the pin geometry. It should be noted that this formalism cannot account for negative values of $\lambda$ or those larger than 1 , as discussed earlier.

### 6.8 Effective Doppler Temperature

(Meghreblian and Holmes 1960, p. 135)

### 6.8.1 Lattice Bonding Effects

For a solid, the velocity distribution of atoms is not strictly a Maxwellian distribution as for a gas, due to the lattice bonds. For instance, the uranium atoms in a $\mathrm{UO}_{2}$

[^113]crystal vibrate at a mean kinetic energy higher than that of a gas of free uranium atoms. These vibrations are quantized since the atoms in the lattice can be considered as being bonded by linear elastic forces. Thus, this quantization is similar to the harmonic oscillator (Born 1971, p. 244). Willis Lamb showed that for weaklybonded atoms, for neutron capture, the latter behave as a free gas with an effective temperature higher than the actual crystal temperature. If the crystal has a group of atoms vibrating at frequency $\nu$ (also known as phonons Egelstaff 1965, p. 28), the quantized state of the crystal shifts by creation or absorption of a phonon when neutrons scatter inelastically (Kittel 1967, p. 137; Born 1971, p. 246). The mean kinetic energy, used to define the effective Doppler temperature, is obtained by integration over all the phonons:
$$
k T_{e f f}=\int_{0}^{\infty} g(\nu) \frac{h \nu}{2} \operatorname{coth}\left(\frac{h \nu}{2 k T}\right) d \nu
$$
where $g(\nu)$ is the phonon distribution. Using the Debye distribution, the following is obtained ${ }^{15}$ :
$$
T_{e f f}=\frac{3}{2} \theta_{\text {Debye }} \int_{0}^{1} x^{3} \operatorname{coth}\left(\frac{x \theta_{\text {Debye }}}{2 T}\right) d x
$$
$\theta_{\text {Debye }}$ is the Debye temperature of the crystal. Using the change of variable $y=x \theta_{\text {Debye }} /(2 T)$, the following equation is reached:
$T_{\text {eff }}=24 \frac{T^{4}}{\theta_{\text {Debye }}^{3}} \int_{0}^{\frac{\theta_{\text {Debye }}}{2 T_{j}}} y^{3} \operatorname{coth}(y) d y$ whence $: \frac{T_{\text {eff }}}{T} \approx 1+\frac{1}{20}\left(\frac{\theta_{\text {Debye }}}{T}\right)^{2}+O\left(\frac{\theta_{\text {Debye }}}{T}\right)^{4}$
The Debye temperature for uranium oxide $\mathrm{UO}_{2}$ was measured precisely by Serizawa et al., ${ }^{16}$ and leads to the cubic empirical formula between 900 K and 1600 K :
$$
\theta_{\text {Debye }_{[K]}}^{\text {OO}_{2}}=1.8910^{-6} T_{[K]}^{3}-6.6710^{-3} T_{[K]}^{2}+7.79 T_{[K]}-2640 .
$$

[^114]Below $1300 K$, the Debye temperature is assumed as being constant: $\theta_{\text {Debye }}^{U O_{2}}=377 \mathrm{~K}$. However, an equivalence for reaction rates leads to effective temperature values far above the Debye temperature, of the order of $620 \mathrm{~K} .{ }^{17}$ This disagreement is due to the fact that the weakly-bonded model is not consistent with reality. Recent studies at $C E A^{18}$ have given the following empirical formula:

$$
\begin{equation*}
\text { Santamarina-Meister formula: } \frac{T_{\text {crystal }}}{T_{\text {eff }}}=1+\frac{8,6}{T_{\text {eff }[K]}}+\frac{3100}{T_{\text {eff }[K]}^{2}} \tag{6.17}
\end{equation*}
$$

This formula accounts for crystalline effects in the $\mathrm{UO}_{2}$ lattice on the Doppler effect. If the fuel temperature is not uniform, the following geometric correction should be used:

$$
T_{e f f}=\overline{T_{\text {fuel }}}+\frac{1}{18}\left(T_{\text {center }}-T_{\text {sulface }}\right)
$$

where $\overline{T_{\text {fuel }}}$ is the mean fuel temperature over its volume, $T_{\text {center }}$ that at its center and $T_{\text {surface }}$ that at its surface. From the last formula, $T_{\text {eff }}$ is defined as an "optical" temperature that takes account of temperature variations along the neutron optical path.

### 6.8.2 Heterogeneity Effects of the Temperature Field

Historically, resonance integral calculations took account of only one temperature in the region containing resonant nuclei. However, temperature has an approximately parabolic variation in the fuel rod. Thus, the temperature to be used as the effective temperature must be chosen properly. It might be trivially supposed that the average medium temperature should be used. The influence of the fuel temperature profile on resonant absorption was studied in 1954 by Roe. ${ }^{19}$ His idea was to model the resonance integral by a unique Breit-Wigner resonance in slab geometry. Roe defined the geometric mean of the first Voigt function as:

[^115]$$
\bar{\psi}=\frac{1}{a} \int_{z=0}^{z=a} \psi(x, \xi(z)) d z
$$
where $z$ is the spatial coordinate along a slab of thickness $a$. Roe then defined the effective temperature as follows:
$$
\int_{x=-\infty}^{x=+\infty} \psi^{2}\left(x, \xi_{e f f}\right) d x=\int_{x=-\infty}^{x=+\infty} \bar{\psi}^{2} d x
$$
where $\xi_{\text {eff }} \equiv \xi\left(T_{\text {eff }}\right)$. He deduced that the effective temperature is approximated for a unique resonance with width $\Gamma$ at energy $E_{0}$ by the formula:
$$
\theta_{e f f}=\bar{\theta}-\frac{3}{2} \frac{\left(\overline{\theta^{2}}-\bar{\theta}^{2}\right)}{1+4 \bar{\theta}} \quad \text { where } \quad \theta(z) \equiv \frac{1}{\xi^{2}}=\frac{4 E_{0} k T(z)}{A \Gamma^{2}}
$$

In 1958, A. Keane ${ }^{20}$ studied the same slab problem, considering only neutrons that are normally incident to the slab and assuming a parabolic fuel temperature profile. He then worked on the following function:

$$
\chi\left(\xi_{\max }, x, \frac{T_{\text {surface }}}{T_{\text {centre }}-T_{\text {sufface }}}\right)=\frac{1}{a} \int_{z=0}^{z=a} \psi(x, \xi(z)) d z
$$

The absorption probability in the slab at reduced energy $x$ is given by the complementary of the non-leakage probability:

$$
P_{a b s}(x)=1-e^{-N \sigma_{0} \int_{z=0}^{z=a} \psi(x, \xi(z)) d z}
$$

For a resonance with high absorption, characterized by $N \sigma_{0} a$, Keane showed that the geometric mean of the fuel temperature $\bar{T}=\left(T_{s}+2 T_{c}\right) / 3$ qualifies correctly as the effective temperature. For low values of $N \sigma_{0} a$, Keane found the same results as Roe.

In 1961, Reichel and Keane studied ${ }^{21}$ this problem for a cylindrical geometry and a parabolic temperature profile:

[^116]$$
T(r)=T_{\text {sufface }}+\frac{\left(R^{2}-r^{2}\right)}{R^{2}}\left(T_{\text {centre }}-T_{\text {sufface }}\right)
$$


A neutron entering the cylinder by the point $O$ and moving along a chord $L$ with curvilinear coordinate $\ell$ experiences the temperature:

$$
T(\ell)=T_{\text {sufface }}+\frac{\left(R^{2}-r^{2}\right) Y^{2}}{R^{2}}\left(T_{\text {center }}-T_{\text {sufface }}\right)\left(\frac{\ell}{L}-\frac{\ell^{2}}{L^{2}}\right)
$$

It can be pointed out that the profile remains parabolic and has a maximum value of:

$$
T_{\max }(Y)=T_{\text {surface }}+\frac{\left(R^{2}-r^{2}\right) Y^{2}}{4 R^{2}}
$$

For a slab of thickness $a$, the parabolic temperature field has the following form:

$$
T(z)=T_{\text {surface }}+\frac{4}{a^{2}}\left(T_{\text {centre }}-T_{\text {surface }}\right)\left(a z-z^{2}\right)
$$

Therefore, a neutron entering the cylinder along the chord $L$ is considered as being perpendicular to a slab of thickness $L$ and with maximum temperature $T_{\max }(Y)$, which allows the definition of an effective temperature of the projected chord $Y$ by analogy:

$$
T_{\text {eff }}(Y)=\frac{1}{3} T_{\text {surface }}+\frac{2}{3} T_{\max }(Y)=T_{\text {surface }}+\frac{Y^{2}}{6 R^{2}}\left(T_{\text {centre }}-T_{\text {surface }}\right)
$$

The distribution of the projected chord $Y$ is such that:

$$
p(Y) d Y=\cos \theta d \theta
$$

$p(Y) d Y$ is the probability of having a projected chord length $Y$ up to $d Y$ for an angle $\theta \in\left[0, \frac{\pi}{2}\right]$.

In 1962, G. Rowlands ${ }^{22}$ proposed that thermalized neutrons have the highest probability of being absorbed in the fuel rod and hence, their spectrum is thermalized. He noticed that if the neutron is not scattered, then it is not influenced by the order of the fuel layers at different temperatures. In this case, an "optical temperature" can be defined by averaging the real temperature crossed for the different chords:

$$
T_{e f f}=\int_{L} \frac{\int_{\ell=0}^{\ell=L} T(\ell) d \ell}{L} p(L) d L
$$

For a slab of thickness $a$, this calculation is extremely simplified provided the temperature field remains parabolic along the chord with a maximum always at the slab center.


L

[^117]\[

$$
\begin{aligned}
T(\ell) & =T_{\text {surface }}+\frac{4}{L^{2} \sin ^{2} \theta}\left(T_{\text {center }}-T_{\text {surface }}\right)\left(L \ell \sin ^{2} \theta-\ell^{2} \sin ^{2} \theta\right) \\
& =T_{\text {sufface }}+\frac{4}{L^{2}}\left(T_{\text {center }}-T_{\text {surface }}\right)\left(L \ell-\ell^{2}\right)
\end{aligned}
$$
\]

Thus, the mean geometric temperature for any chord $L$ is always given by:

$$
T_{\text {eff }}(L)=\frac{1}{3} T_{\text {surface }}+\frac{2}{3} T_{\text {center }}
$$

The probability of having a chord $L$ in a slab of thickness $a$ is given by:

$$
p(L) d L=\frac{2 a^{2}}{L^{3}} d L
$$

where:

$$
\begin{aligned}
T_{\text {eff }} & =\int_{L}^{\ell=L} \frac{\int_{\ell=0}^{\ell=L} T(\ell) d \ell}{L} p(L) d L=\int_{L=a}^{L=+\infty}\left(\frac{1}{3} T_{\text {suface }}+\frac{2}{3} T_{\text {center }}\right) p(L) d L \\
& =\frac{1}{3} T_{\text {surface }}+\frac{2}{3} T_{\text {center }}
\end{aligned}
$$

The optical temperature coincides with the mean geometrical temperature for a slab.

Assuming that Rowlands' idea that any temperature distribution with a wellchosen order can be reduced to a parabola is equivalent to this very parabola, and that the effective temperature along the chord is reduced to the computation of the optical temperature, an analytical calculation can be carried out for a cylinder:

$$
T_{\text {eff }} \equiv \int_{Y=0}^{Y=2 R} \overline{T(Y)} p(Y) d Y=\frac{5}{9} T_{\text {surface }}+\frac{4}{9} T_{\text {center }}
$$

It can be seen that for a cylinder, the mean geometric temperature $\left(T_{\text {surface }}+T_{\text {center }}\right) / 2$ is no longer obtained.

In 1979, based on numerical considerations, Basiuk, Reuss, Tellier and Van der Gucht from CEA calculated the coefficients to be applied to the temperatures at the center and at the surface of the fuel rod so as to correctly compute absorption rates, assuming a parabolic temperature profile (Table 6.4). It should be noted that a parabolic temperature profile in the fuel rod means that the heat equation has been integrated with a constant power per unit volume term. Actually, this never occurs in practice since the production of ${ }_{94}^{239} \mathrm{Pu}$ at the fuel rod surface due to preferential

Table 6.4 Effective weighting of surface and center temperatures for the Doppler effect

| Geometry | Volume average | Rowlands | Basiuk-Reuss-Tellier- <br> Van der Gucht |
| :--- | :--- | :--- | :--- |
| Cylinder | $\frac{1}{2} T_{s}+\frac{1}{2} T_{c}$ | $\frac{5}{9} T_{s}+\frac{4}{9} T_{c}$ | $0.549 T_{s}+0.451 T_{c}$ |
| Slab | $\frac{1}{3} T_{s}+\frac{2}{3} T_{c}$ | $\frac{1}{3} T_{s}+\frac{2}{3} T_{c}$ | $0.235 T_{s}+0.765 T_{c}$ |
| Sphere | $\frac{3}{5} T_{s}+\frac{2}{5} T_{c}$ | $\frac{2}{3} T_{s}+\frac{1}{3} T_{c}$ | $0.662 T_{s}+0.318 T_{c}$ |

absorption by ${ }_{92}^{238} U$ leads to a pronounced depression within the rod, known as a rim effect. This phenomenon worsens with burnup.

After working on the matter, Paul Reuss estimated that the error induced by assuming a parabolic temperature profile is much greater than the discrepancy due to the different formulations. Hence, Rowlands' formula continues to be widely used for industrial applications.

## Chapter 7 <br> Thermalization of Neutrons

Neutrons reach thermal energy following successive collisions with moderator nuclides provided they are neither absorbed nor leak out of the reactor. At this point, they can either lose energy by collision or gain energy if the target nucleus is itself in thermal motion, and can thus transfer momentum to the neutrons. Hence, an equilibrium state is obtained whereby neutrons may be assimilated as a gas of weak density, in which velocities are characterized by the moderator temperature.
(Reactor Physics 1966, volume 1)

### 7.1 Historical Background

The apparently disorderly motion of molecules in a gas at a given temperature is amplified as the temperature increases. The word gas was itself coined around 1643 by Flemish alchemist doctor, Jan Baptist Van Helmont, from a Latin word meaning "chaos". The agitated motion was first described in scientific terms by botanist Robert Brown (1773-1858), director of the British Museum in 1827. He described the intense and disorderly Brownian motion of pollen grains in suspension in a closed room, before examining them closely in solution under a microscope (Bloch 1958, p93). He soon concluded that the motion was not due to fluid currents or progressive evaporation, but that it came from the particles themselves. But what was the cause? The phenomenon became known by his name: Brownian motion. In 1860, the kinetic theory of gases described by James Clerk Maxwell ${ }^{1}$ provided an explanation for this phenomenon (Génie de la science n${ }^{\circ} 24$ 2005) (Photo 7.1).

[^118]Photo 7.1 James Clerk Maxwell (1831-1879) produced major works on electromagnetism, heat theory and kinetic theory of gases during his 48 years (Public domain)


It describes the behavior of a large number of gas molecules. Maxwell was familiar with statistics and used that powerful mathematical tool to determine the speed distribution of molecules around the mean speed. His calculations led to a microscopic explanation for the ideal gas equation $P V=n R T$ (it should be pointed out that at that time, the hypothesis of the existence of molecules was not widely accepted).

### 7.2 Boltzmann Theory of Gases

(Boltzmann 1902; Vassiliev 1985)
In 1872, Ludwig Boltzmann ${ }^{2}$ statistically demonstrated the distribution law for the velocities of gas molecules discovered in 1860 by Maxwell, and he interpreted the notion of entropy by linking it to probability (the probabilistic approach of

[^119]thermodynamics in 1877). The Boltzmann distribution (1896) showed that the number of particles of energy $E$ in an elementary volume $d^{3} r$ of a total volume $V$ is proportional to the volume and varies as a negative exponential function with energy (Born 1971, p21; Jouguet 1964, p91]:
$$
n(E, \vec{r}) d r^{3}=\alpha e^{-\beta E} \frac{d^{3} r}{V}
$$

For an ideal monatomic gas (i.e. the potential interaction energy between the molecules themselves is negligible compared to their kinetic energy, given by $E=m v^{2} / 2$ ), the coefficients $\alpha$ and $\beta$ are obtained by normalizing with respect to the total number of molecules $n$ in the total volume and the average total energy of the system $E_{\text {tot }}$. It is thus necessary to first define the elementary integration volume in the phase space [Diu et al. 2001, p82 and p239]. The integration with respect to energy $E=m\left(v_{x}^{2}+v_{y}^{2}+v_{z}^{2}\right) / 2$ is equivalent to integrating over the differential speed elements $d v_{x} d v_{y} d v_{z}$ ):

$$
\begin{aligned}
n_{\text {tot }} & =\int_{\substack{v_{x}=-\infty \\
v_{x}=+\infty}}^{v_{x}=+\infty} \int_{\substack{v_{y}=-\infty}}^{v_{y}=+\infty} \int_{V}^{v_{y}=+\infty} n(E, \vec{r}) d^{3} r \\
& =\int_{v_{x}=-\infty}^{v_{z}=+\infty} d v_{x} \int_{v_{y}=-\infty}^{v_{z}=+\infty} d v_{y} \int_{v_{z}=-\infty} d v_{z} \iint_{x} \int_{y} \alpha e^{-\beta \frac{1}{2} m\left(v_{x}^{2}+v_{y}^{2}+v_{z}^{2}\right)} \frac{d x d y d z}{V}
\end{aligned}
$$

Integration over the volume is obtained directly. Integration with respect to velocities can be carried out either by an integral on the sphere of velocities (where $v$ is the radius for the polar integral term), or by noticing that the variables $v_{x}, v_{y}$ and $v_{z}$ are independent, hence leading to computation of the integral by breaking it down into three integrals through the exponential term, as shown below:

$$
n_{t o t}=\alpha \underbrace{\int_{v_{x}=-\infty}^{v_{x}=+\infty} d v_{x} e^{-\beta \frac{1}{2} m v_{x}^{2}}}_{\sqrt{\frac{2 \pi}{p m}}} \int_{v_{y}=-\infty}^{v_{y}=+\infty} d v_{y} e^{-\beta \frac{1}{2} m v_{y}^{2}} \int_{v_{z}=-\infty}^{v_{z}=+\infty} d v_{z} e^{-\beta_{2}^{1} m v_{z}^{2}}=\alpha\left(\frac{2 \pi}{\beta m}\right)^{\frac{3}{2}}
$$

The average total energy is computed using integration over the sphere of velocities for didactic purposes:

$$
\begin{aligned}
E_{\text {tot }}=\int_{v_{x}=-\infty}^{v_{x}=+\infty} \int_{v_{y}=-\infty}^{v_{y}=+\infty} \int_{v_{z}=-\infty}^{v_{z}=+\infty} \int_{V} \frac{1}{2} m v^{2} n(E, \vec{r}) d^{3} r=\int_{v=0}^{v=+\infty} d v 4 \pi v^{2} \alpha \frac{1}{2} m v^{2} e^{-\beta \frac{1}{2} m v^{2}} \\
=2 \pi m \alpha \underbrace{\int_{v=0} d v v^{4} e^{-\beta \frac{1}{2} m v^{2}}}_{v=+\infty} \\
\frac{\frac{1}{2} \Gamma\left(\frac{5}{2}\right) /\left(\frac{\beta m}{2}\right)^{\frac{5}{2}}}{l}
\end{aligned}
$$

where:

$$
E_{t o t}=\frac{3}{4} m \alpha \sqrt{\frac{\pi^{3}}{\left(\frac{\beta m}{2}\right)^{5}}}=\frac{3}{2} \frac{n_{t o t}}{\beta}
$$

Statistical thermodynamics indicates that, on average, each degree of freedom for a single molecule has an energy of $k T / 2$. A free molecule has three degrees of freedom in space, i.e. $3 k T / 2$ of average total energy (Bloch 1958, p95). Therefore, we have:

$$
\beta=\frac{1}{k T} \text { and } \alpha=n\left(\frac{m}{2 \pi k T}\right)^{\frac{3}{2}}
$$

The speed distribution is called the Maxwell distribution. For a gas of identical molecules of mass $m$ at temperature $T$, it is written as (Diu et al. 2001; Stacey 2001, p104; Vassiliev 1985, p80):

$$
n(v) d v=4 \pi\left(\frac{m}{2 \pi k T}\right)^{3 / 2} v^{2} e^{-\frac{m v^{2}}{2 k T}} d v
$$

where:

$$
n(v) d v=\frac{4}{\sqrt{\pi}} \frac{v^{2}}{\left(\frac{2 k T}{m}\right)^{\frac{3}{2}}} e^{-\frac{\frac{1}{2} m v^{2}}{k T}} d v=\frac{4}{\sqrt{\pi}} \frac{v^{2}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{2}}} d v
$$

where $k=1.38054 \times 10^{-23} \mathrm{~J} \mathrm{~K}^{-1}$ is the Boltzmann constant (Photo 7.2).
$v_{T}=\sqrt{2 k T / m}$ is the most probable speed at energy $k T$. Since kinetic energy is equal to $E=m v^{2} / 2$, where $d E=m v d v, n(E) d E$ can be computed by substituting $v$ by $\sqrt{2 E / m}$. The equation for the distribution of velocities should be compared with the classical mathematical equation for a Maxwell distribution:

Photo 7.2 Ludwig
Boltzmann was a great though very tormented physicist. In 1906, he committed suicide since his theories were not widely understood (Public domain)


$$
m_{\sigma}(x)=\frac{1}{\sigma \sqrt{2 \pi}} e^{-\frac{(x-\bar{m})^{2}}{2 \sigma^{2}}}
$$

where the mean value is $\bar{m}$, the standard deviation is $\sigma$ and the variance is $\sigma^{2}$. The distribution in terms of speed is transformed into distribution in terms of energy (Jouguet 1964, p100):

$$
n(v) d v=4 \pi\left(\frac{m}{2 \pi k T}\right)^{3 / 2} v^{2} e^{-\frac{E}{k T}} \frac{d E}{m v}=4 \pi\left(\frac{m}{2 \pi k T}\right)^{3 / 2} \sqrt{\frac{2 E}{m^{3}}} e^{-\frac{E}{k T}} d E
$$

Which leads to distribution in molecular energy, denoted $n(E)^{3}$ :

$$
n(E) d E=4 \pi \frac{m}{2 \pi k T} \sqrt{\frac{m}{2 \pi k T}} \sqrt{\frac{2 E}{m}} \frac{1}{m} e^{-\frac{E}{k T}} d E=\frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} e^{-\frac{E}{k T}} \frac{d E}{k T}
$$

with normalization to unity verified through calculation as:

$$
\int_{0}^{\infty} n(v) d v=\int_{0}^{\infty} n(E) d E=\int_{0}^{\infty} \frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} e^{-\frac{E}{k T}} \frac{d E}{k T}=\frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}\right)=1
$$

Sometimes, neutron density is expressed using the reduced speed $x=v / v_{T}$, giving the following expression:

[^120]Distribution of thermal neutrons : $n(v) d v$

$$
\begin{equation*}
=\frac{4}{\sqrt{\pi}} \frac{v^{2}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{2}}} d v=\frac{4}{\sqrt{\pi}} x^{2} e^{-x^{2}} d x=n(x) d x \tag{7.1}
\end{equation*}
$$

### 7.3 Application to Neutrons

(Neutron fluence measurements 1970, p45; Progress in nuclear energy Vol 2 1958, p91)

As the neutron slows down, the kinetic energy of target nuclides due to thermal agitation at temperature $T$ for the non-absorbing moderating medium cannot be neglected anymore. Neutrons will thus ultimately have the same speed spectrum as the medium in which they propagate. As the number of neutrons in a reactor is very small, ${ }^{4}$ collision between neutrons may be disregarded. At equilibrium, it is assumed that neutrons have the same speed field as the target nuclides they collide. Hence, the mean gain in lethargy per collision is zero, while during slowing-down, it was $\xi=1-\frac{\alpha}{1-\alpha} \log \frac{1}{\alpha}$. A continuous link describes transit from the purely slowing-down zone to the so-called thermalization zone (Fig. 7.1).


Fig. 7.1 Link between the slowing-down and thermalization zones

[^121]This would be accurate if no neutron absorption occurred. Absorption can in fact be viewed as a leakage term that leads to loss of neutrons at certain velocities only, mostly due to resonances. If absorption is weak, and by analogy with a gas, the neutron density distribution in terms of energy is given by:

$$
n(E) d E=n_{t h} \frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} e^{-\frac{E}{k T}} \frac{d E}{k T}
$$

where:
$n(E)$ is the number of neutrons at energy $E$ per unit volume and energy [neutrons/ $\left.\mathrm{cm}^{3} / \mathrm{eV}\right]$.
$n_{t h}$ is the normalization coefficient [neutrons $/ \mathrm{cm}^{3}$ ].
$T$ is the moderator temperature [K]: by analogy with a gas, it will be called the neutron temperature with great caution in order to avoid all potential confusion.

This is the Maxwell distribution or Maxwell spectrum. In theory, this distribution is valid only for a non-absorbing medium. For slightly absorbing moderators, the thermal spectrum is shifted towards higher energies since absorption increases at low energy. This effect is often neglected in light water reactors. Distribution can be readily expressed in terms of speed by denoting $n(E) d E=n(v) d v$ :

$$
n(E) d E=\frac{2}{\sqrt{\pi}} n_{t h} \sqrt{\frac{\frac{1}{2} m v^{2}}{k T}} e^{-\frac{\frac{1}{2} m v^{2}}{k T}} \frac{m v d v}{k T}=n_{t h} \frac{4}{\sqrt{\pi}} \sqrt{\frac{m}{2 k T}} \frac{\frac{1}{2} m v^{2}}{k T} e^{-\frac{1}{2} m v^{2}} k
$$

where:

$$
n(v)=n_{t h} \frac{4}{\sqrt{\pi}} \sqrt{\frac{m}{2 k T}} \frac{\frac{1}{2} m v^{2}}{k T} e^{-\frac{1}{2} \frac{m v^{2}}{k T}}=n_{t h} \frac{4}{\sqrt{\pi}} \frac{v^{2}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{2}}}
$$

The normalization factor is such that $\int_{0}^{\infty} n(v) d v=n_{t h}$ since:

$$
\int_{0}^{\infty} x^{2} e^{-x^{2}} d x=\frac{\sqrt{\pi}}{4} \quad \text { et } \quad \int_{0}^{\infty} \sqrt{x} e^{-x} d x=\frac{\sqrt{\pi}}{2}=\Gamma\left(\frac{3}{2}\right)
$$

where $\Gamma$ is the real factorial (Erdélyi et al. 1953, p1). The most probable neutron speed $v_{T}$ (of mass $m=1.6749286 \times 10^{-17} \mathrm{~kg}$ ) for the Maxwell distribution at temperature $T$ corresponds to the maximum value of $n(v)$ (i.e. where the derivative of $n(v)$ is zero):

$$
\frac{1}{2} m v_{T}^{2}=k T \quad \text { i.e. } \quad v_{T}=\sqrt{\frac{2 k T}{m}}=\sqrt{\frac{T}{T_{0}}} v_{0}
$$

Table 7.1 Maxwell distribution of velocities $T=579.15 \mathrm{~K}=306^{\circ} \mathrm{C}$

| $v_{\left[\mathrm{m} \mathrm{s}^{-1}\right]}$ | 0 | 1000 | 2200 | 3090 | 4000 | 6000 | 10,000 | 20,000 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $m(v)_{\left[\text {neutron } /\left(\mathrm{m} \mathrm{s}^{-1}\right)\right]}$ | 0 | $6.889 \times 10^{-5}$ | $2.230 \times 10^{-4}$ | $2.687 \times 10^{-4}$ | $2.291 \times 10^{-4}$ | $6.344 \times 10^{-5}$ | $2.161 \times 10^{-7}$ | $1.950 \times 10^{-20}$ |



Fig. 7.2 Plot of Maxwell speed distribution for $T=579.15 \mathrm{~K}=306^{\circ} \mathrm{C}$
For $T=579.15 \mathrm{~K}\left(306^{\circ} \mathrm{C}\right) \quad v_{579 \mathrm{~K}}=3090 \mathrm{~m} \cdot \mathrm{~s}^{-1} \quad E_{579 \mathrm{~K}}=0.05 \mathrm{eV}$
For $T=T_{0}=293.59 \mathrm{~K}\left(20.44^{\circ} \mathrm{C}\right) \quad v_{293 \mathrm{~K}}=v_{0}=2200 \mathrm{~m} \cdot \mathrm{~s}^{-1} \quad E_{293 \mathrm{~K}}=E_{0}=0.0253 \mathrm{eV}$
For $T=273.15 \mathrm{~K}\left(0^{\circ} \mathrm{C}\right) \quad v_{273 \mathrm{~K}}=2122 \mathrm{~m} \cdot \mathrm{~s}^{-1} \quad E_{273 \mathrm{~K}}=0.0235 \mathrm{eV}$
It should be pointed out that the conventional notations $v_{0}$ and $E_{0}$ correspond to a temperature not of $0^{\circ} \mathrm{C}$ but rather of $20.44^{\circ} \mathrm{C}$. A particularly useful Maxwell distribution is that for water temperature in the vessel of a $P W R$, i.e. $306^{\circ} \mathrm{C}$, certain values of which are given in Table 7.1 and plotted in Fig. 7.2.

The average speed of distribution $\bar{v}$, not to be confused with the most probable speed $v_{T}$, is given by:

$$
\bar{v} \equiv \frac{\int_{0}^{\infty} v n(v) d v}{\int_{0}^{\infty} n(v) d v}=\sqrt{\frac{8 k T}{\pi m}}=\frac{2}{\sqrt{\pi}} v_{T}=\frac{1}{0.886} v_{T}
$$

For $T=T_{0}=20.44^{\circ} \mathrm{C}$ (laboratory reference), $\quad \bar{v}=2482.4 \mathrm{~m} \mathrm{~s}^{-1}$.
For $T=306^{\circ} \mathrm{C}(P W R), \quad \bar{v}=3487.6 \mathrm{~m} \mathrm{~s}^{-1}$.
This result is obtained using the neutron density distribution with speed:

$$
\begin{aligned}
\bar{v} & =\frac{\int_{0}^{\infty} v n(v) d v}{\int_{0}^{\infty} n(v) d v}=\frac{\int_{0}^{\infty} v n_{t h} \frac{4}{\sqrt{\pi}} \frac{v^{2}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{2}}} d v}{n_{t h}}=\frac{4}{\sqrt{\pi}} \int_{0}^{\infty} \frac{v^{3}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{2}}} d v \\
& =\frac{4}{\sqrt{\pi}} v_{T} \int_{0}^{\infty} x^{\frac{3}{2}} e^{-x} \frac{d x}{2 \sqrt{x}}
\end{aligned}
$$

thus:

Mean speed for a Maxwell distribution: $\bar{v}=\frac{2}{\sqrt{\pi}} v_{T} \underbrace{\Gamma(2)}_{1}=\frac{2}{\sqrt{\pi}} v_{T}$
The most probable speed $v_{T}$ and the average speed are related by the following formula: $\bar{v}=2 v_{T} / \sqrt{\pi}$.

$$
\begin{equation*}
\text { Most probable speed: } v_{\mathrm{T}}=\frac{\sqrt{\pi}}{2} \bar{v}=\sqrt{\frac{T}{T_{0}} v_{0}} \tag{7.3}
\end{equation*}
$$

The most probable energy occurs for the largest neutron density $n(E)$. It is worth $E=k T / 2$ for a Maxwell distribution. The mean energy of the distribution is equal to $\bar{E}=3 k T / 2=3 E_{T} / 2$ with $E_{T}=k T=m v_{T}^{2} / 2$.

### 7.4 Neutron Flux Spectrum

The flux spectrum is the product of the neutron density with the speed of these neutrons:

$$
\Phi(E)=m(E) \quad v(E)=m(E) \sqrt{\frac{2 E}{m}} \quad \text { or }: \quad \Phi(E)=n_{t h} \sqrt{\frac{8 k T}{\pi m}} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}
$$

The Maxwell function or Maxwell distribution of the function $m(E)$ is such that:

$$
\begin{equation*}
\text { Maxwell function in terms of energy: } m(E) \equiv \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}} \text { in }\left[\mathrm{eV}^{-1}\right] \tag{7.4}
\end{equation*}
$$

The function verifies the following normalization $\int_{0}^{\infty} m(E) d E=1$ since $\int_{0}^{\infty} y e^{-y} d y=1$, by adopting the change in variable given by $y=E / k T$. Using the reduced variable $x \equiv v / v_{T}$, the result is:

$$
\begin{equation*}
\text { Maxwell function with reduced speed: } m(x) d x=\frac{4}{\sqrt{\pi}} x^{2} e^{-x^{2}} d x \tag{7.5}
\end{equation*}
$$

The integrated thermal flux is the quantity given by:

$$
\begin{align*}
& \text { Thermal neutron flux: } \Phi_{t h}=\int_{0}^{\infty} \Phi(E) d E \\
& \qquad=\sqrt{\frac{8 k T}{\pi m}} n_{t h} \underbrace{\int_{0}^{\infty} m(E) d E}_{1}=n_{t h} \sqrt{\frac{8 k T}{\pi m}}=n_{t h} \bar{v} \tag{7.6}
\end{align*}
$$

The units are those for a flux that is the product of neutron density and speed.
With $\Phi_{t h} \approx 3 \times 10^{13} \mathrm{n} . \mathrm{cm}^{-2} . \mathrm{s}^{-1}, T_{\mathrm{H}_{2} \mathrm{O}}=300^{\circ} \mathrm{C}=573.15 \mathrm{~K}, k=1.38054 \times 10^{-23}$ J. $\mathrm{K}^{-1}, m_{\text {neutron }}=1.67 \times 10^{-27} \mathrm{~kg}$, the following value is obtained: $n_{\text {th }}=8.63 \times 10^{7}$ neutrons $\mathrm{cm}^{-3}$

If this neutron density is compared to that of an ideal gas for instance, 1 mole of the latter at a pressure of 1 atmosphere and a temperature of 293 K has a volume of 22.4 i.e. $22.4 \times 10^{3} \mathrm{~cm}^{3}$, equivalent to a molecular density of:

$$
\frac{6.022 \times 10^{23}}{22.4 \times 10^{3}}=2.7 \times 10^{19} \text { molecule } / \mathrm{cm}^{3}
$$

It may be seen that thermal neutrons form a gas of very low density: the notion of an ideal gas applied to neutrons is therefore valid, as is the notion that collision between two neutrons is highly unlikely. The latter point is very important since a neutron gas is at thermal equilibrium, with a Maxwell distribution of speeds, due to the collision of neutrons with "hot" matter, and not with other neutrons, as is the case for a gas with collisions between molecules.

In a thermal reactor, the matter referred to earlier is the moderator since the (heavy) fuel contributes weakly to the slowing down of neutrons. Contrary to common belief, very few neutrons are present in a reactor at any given time. It should be noted that the maximum flux spectrum in energy occurs at $E=k T$, which is the most probable energy, whereas the maximum of the neutron spectrum occurs at $E=k T / 2$ (Fig. 7.3 and Table 7.2)

$$
\frac{d \Phi(E)}{d E}=\Phi_{t h}\left(\frac{1}{(k T)^{2}}-\frac{E}{(k T)^{3}}\right) e^{-\frac{E}{k T}} \quad \frac{d n(E)}{d E}=n_{t h} \frac{2}{\sqrt{\pi}} \sqrt{\frac{1}{k T}} \frac{e^{-\frac{E}{k T}}}{k T}\left(\frac{1}{2 \sqrt{E}}-\frac{\sqrt{E}}{k T}\right)
$$



Fig. 7.3 Comparison of neutron density and flux spectrum as a function of energy

Table 7.2 Maxwell distribution in energy for $T=579.15 \mathrm{~K}=306^{\circ} \mathrm{C}$

| $v_{\left[\mathrm{m}^{-1}\right]}$ | 0 | 1000 | 2200 | 3090 | 4000 | 6000 | 10000 | 20,000 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $E / k T_{[-]}$ | 0 | 0.1 | 0.5 | 1 | 1.68 | 3.77 | 10.50 | 41.90 |
| $n(E)_{\left[\text {neutron } \mathrm{J}^{-1}\right]} \times 10^{19}$ | 0 | 5.4 | 6.1 | 5.2 | 3.4 | 0.63 | 0.0013 | $5.8 \times 10^{-17}$ |
| $\Phi(E)_{\left[\text {neutron } \mathrm{cm}^{-2} \mathrm{~s}^{-1} \mathrm{~J}^{-1}\right]} \times 10^{19}$ | 0 | 2.3 | 3.8 | 4.6 | 3.9 | 1.1 | 0.0037 | $3.3 \times 10^{-16}$ |

### 7.5 Neutron Thermalization Equation

(Neutron thermalization 1962)
When neutrons reach thermal energy, they may either lose or gain energy through collision. The thermalization equation is very similar to the slowingdown equation, the difference being that integration over energy is done over [ 0 , $+\infty[$ rather than limiting the range of the scattering rate to $E$.

$$
\underbrace{\int_{0}^{\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(E^{\prime}\right) d E^{\prime}}=\underbrace{\Sigma_{t}(E) \Phi(E)}
$$

(1) Neutrons which arrive at energy $E$ up to $d E$ from $E^{\prime}$
(2) Neutrons
which disappear

It may be seen that there is no fission source term since the neutrons are always emitted in the fast energy range. If there is no absorption and the medium has no leakage, the Maxwell function $m(E)$ is in fact the solution to the thermalization equation (7.7) (Fig. 7.4).

The scattering cross section can be introduced into the neutron loss term on the RHS of the equation:

Thermalization equation: $\int_{0}^{\infty} \Sigma_{S}\left(E^{\prime} \rightarrow E\right) \Phi\left(E^{\prime}\right) d E^{\prime}=\Sigma_{a}(E) \Phi(E)$

$$
+\underbrace{\Sigma_{S}(E)}_{\int_{0}^{\infty} \Sigma_{S}\left(E-E^{\prime}\right) d E^{\prime}} \Phi(E)
$$

Furthermore, application of the micro-reversibility principle of Tolman ${ }^{5}$ and the detailed balance (after Fowler and Milne, ${ }^{6}$ which lead to the Onsager reciprocity equations in thermodynamics) to the neutron gas at equilibrium relates at thermal

[^122]Fig. 7.4 Neutron balance at energy $E$

equilibrium the probabilities of scattering from energy $E$ to $E^{\prime}$ and vice versa (Squires 1996, p68; Decoster et al. 1998, p142):

Number of collisions $(E) P\left(E \rightarrow E^{\prime}\right)=$ Number of collisions $\left(E^{\prime}\right) P\left(E^{\prime} \rightarrow E\right)$.
From which:

$$
n(E) v(E) \Sigma_{s}\left(E \rightarrow E^{\prime}\right)=n\left(E^{\prime}\right) v\left(E^{\prime}\right) \Sigma_{s}\left(E^{\prime} \rightarrow E\right)
$$

This approach also enables proper definition of thermal energy by stating that at that particular energy, a neutron has an equal probability of gaining energy or of losing energy. Ideal thermalization implicitly means that there is no absorption, which is not the case in true physical media. A thermalization operator $H$ is introduced, such that:

$$
H[\Phi(E)]=\int_{0}^{\infty} \Sigma_{S}\left(E^{\prime}, E\right) \Phi\left(E^{\prime}\right) d E^{\prime}-\Phi(E) \int_{0}^{\infty} \Sigma_{S}\left(E, E^{\prime}\right) d E^{\prime}
$$

The thermalization equation is hence written as:

$$
H[\Phi(E)]=\Sigma_{a}(E) \Phi(E)
$$

V.V. Smelov, cited in (Marchuk 1959), proposed ${ }^{7}$ expansion of the scattering cross section in terms of the relative velocity between the neutron ( $\vec{v}$ ) and its target ( $\vec{V}$ ):

$$
\Sigma_{s}\left(v_{r}=|\vec{v}-\vec{V}|\right)=\sum_{i} \Sigma_{i} e^{-\alpha_{i} v_{r}^{2}}
$$

This form allows analytical integration of the scattering probability for a monatomic gas of target particles:

[^123]$$
g\left(\vec{\Omega} \rightarrow \overrightarrow{\Omega^{\prime}}, \vec{v} \rightarrow \overrightarrow{v^{\prime}}\right)=\frac{1}{4 \pi} \int_{0}^{2 \pi} d \phi \int_{-1}^{+1} d \mu \int_{0}^{\infty} d v_{r} m(V) p\left(\vec{v} \rightarrow \overrightarrow{v^{\prime}}, \vec{V}\right)
$$
where $m(V)$ is the Maxwell distribution of the speeds of the target nuclides, $p\left(\vec{v} \rightarrow \overrightarrow{v^{\prime}}, \vec{V}\right)$, the probability of reaching velocity $\overrightarrow{v^{\prime}}$ after a collision at velocity $\vec{v}$ with a target (velocity $\vec{V}$ ) and $\mu$ is the cosine of the angle between the velocity before collision and the velocity of the target, while $\mu_{0}$ is that between the velocity after collision and the velocity of the center of mass.
$v_{\min }=\left|\frac{A}{1+A} v_{r}-v_{\text {com }}\right|$ the minimum velocity that can be reached after collision, $v_{\max }=\frac{A}{1+A} v_{r}+v_{\text {com }}$ the maximum velocity that can be reached after collision, $\vec{v}_{\text {com }}=\frac{\vec{v}+A \vec{V}}{1+A}$ is the velocity of the center of mass before collision, $\kappa=\frac{A}{1+A} \frac{v_{r}}{v_{\text {com }}}$ Scattering probability in velocity :
\[

p\left(\vec{v} \rightarrow \overrightarrow{v^{\prime}}, \vec{V}\right)=\left\{$$
\begin{array}{l}
0 \quad \text { if } v^{\prime}<v_{\min }  \tag{7.8}\\
\frac{1}{2 \pi} \frac{2 v^{\prime}}{v_{\max }^{2}-v_{\min }^{2}} \delta\left(\frac{\kappa+1}{2} \frac{v}{v_{\min }}-\frac{\kappa+1}{2} \frac{v_{\min }}{v}-\mu_{0}\right) \quad \text { if } \quad v_{\min } \leq v^{\prime} \leq v_{\max } \\
0 \quad \text { if } v^{\prime}>v_{\max }
\end{array}
$$\right.
\]

The Kronecker delta indicates that only the angle defined by the cosine $\mu_{0}$ may be reached after collision (up to an azimuthal symmetry around the velocity vector of the center of mass). Integration of the previous equation was carried out by Maiorov and Smelov for any mass number and leads to:

$$
\begin{gathered}
g\left(\vec{\Omega} \rightarrow \overrightarrow{\Omega^{\prime}}, \vec{v} \rightarrow \overrightarrow{v^{\prime}}\right)=\frac{(1+A)^{2}}{4 A} \frac{\beta}{\sqrt{A \pi^{3}}\left|\overrightarrow{v^{\prime}}-\vec{v}\right|} \sum_{i} \Sigma_{i} \tau_{i}^{2} e^{-\theta_{i}} \\
\text { with }: \theta_{i} \equiv \alpha_{i} \tau_{i}^{2} v^{\prime 2}-\frac{\left(\alpha_{i}+A \beta^{2}\right)}{4}\left[\frac{\left|\overrightarrow{v^{\prime}}-\vec{v}\right|}{A} \lambda_{i}-\tau_{i}^{2} \frac{v^{2}-v^{\prime 2}}{\left|\overrightarrow{v^{\prime}}-\vec{v}\right|}\right]^{2}, \beta \equiv \frac{1}{\sqrt{2 k T}}, \tau_{i}^{2} \equiv \frac{A \beta^{2}}{\alpha_{i}+A \beta^{2}} \\
\lambda_{i} \equiv 1+A\left(1-\tau_{i}^{2}\right)
\end{gathered}
$$

The scattering probability appears directly in the thermalization equation written as follows:

$$
\begin{aligned}
& \frac{1}{v} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, v, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, v, t)+\Sigma_{t} \Phi(\vec{r}, \vec{\Omega}, v, t) \\
= & \int_{0}^{v_{\text {lhres }}} d v^{\prime} \int d \vec{\Omega}^{\prime} \Phi\left(\vec{r}, \vec{\Omega}^{\prime}, v^{\prime}, t\right) \frac{g\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}, \overrightarrow{v^{\prime}} \rightarrow \vec{v}\right)}{v^{\prime}}+S(\vec{r}, \vec{\Omega}, v, t)
\end{aligned}
$$

$v_{\text {thres }}$ is the speed corresponding to the threshold energy $E_{\text {thres }}$ below which the collisions are assumed to be elastic, since this approach is not valid for inelastic collisions. The integral term thus represents the contribution of those neutrons undergoing elastic scattering out of the total scattering. In the thermalization zone, the fission source term can legitimately be disregarded, unlike the slowingdown source $S(\vec{r}, \vec{\Omega}, E, t)$ for neutrons that are slowed down at energy $E$ below the threshold energy. The integral of the slowing-down source $S(\vec{r}, \vec{\Omega}, t)$ over [0, $\left.E_{\text {thres }}\right]$ corresponds to the total number of neutrons scattering above the threshold value, i.e. the angular slowing-down density at the threshold:

$$
\left\{\begin{array}{rl}
S(\vec{r}, \vec{\Omega}, E, t) & =\int_{E_{\text {trres }}}^{+\infty} d E^{\prime} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, E^{\prime} \rightarrow E, t\right) \Phi\left(\vec{r}, \vec{\Omega}, E^{\prime}, t\right) \\
S(\vec{r}, \vec{\Omega}, t) & =\int_{0}^{E_{\text {thres }}} S(\vec{r}, \vec{\Omega}, E, t) d E=q\left(\vec{r}, \vec{\Omega}, E_{\text {thres }}, t\right) \\
& =\int_{E_{\text {thres }}}^{+\infty} d E^{\prime} \int_{0}^{E_{\text {coup }}} d E^{\prime \prime} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, E^{\prime} \rightarrow E^{\prime \prime}, t\right) \Phi\left(\vec{r}, \vec{\Omega}, E^{\prime}, t\right)
\end{array} .\right.
$$

Integration of the previous differential equation for speeds lower than the threshold speed gives the following equation:

Transport equation at thermal energy:
$\frac{1}{v_{T}} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, t)+\Sigma_{t, T} \Phi(\vec{r}, \vec{\Omega}, v, t)=\int d \vec{\Omega}^{\prime} \Sigma_{s, T} \Phi\left(\vec{r}, \vec{\Omega}^{\prime}, t\right) g\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right)+S(\vec{r}, \vec{\Omega}, t)$
using the fact that for no absorption and leakage, the flux spectrum has a Maxwell distribution similar to the targets with which it is in equilibrium:

$$
\Phi\left(\vec{r}, \vec{\Omega}^{\prime}, v^{\prime}, t\right)=\Phi\left(\vec{r}, \overrightarrow{\Omega^{\prime}}, t\right) m\left(v^{\prime}\right)
$$

taking the thermal scattering reaction rate as:

$$
\Sigma_{s, T} g\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \equiv \int_{0}^{v_{\text {thres }}} d v \int_{0}^{v_{\text {thres }}} d v^{\prime} m\left(v^{\prime}\right) \frac{g\left(\vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, \overrightarrow{v^{\prime}} \rightarrow \vec{v}\right)}{v^{\prime}}
$$

and the average speed at the temperature $T$ as: $v_{T} \equiv\left(\int_{0}^{v_{\text {vilres }}} d v \frac{m(v)}{v}\right)^{-1}$
Equation (7.9) is simply the neutron transport equation condensed on the thermal energy group, and which will be discussed in detail in the chapter on the Bolzmann equation.

### 7.6 Wigner-Wilkins Model: Free Proton Gas

E.P. Wigner and J.E. Wilkins proposed a thermalization model resulting from the collision of neutrons with protons of same mass, without any chemical bonding, and with an absorption cross section inversely proportional to speed. The authors were manifestly seeking to model slowing-down in water while neglecting oxygen, hence the notion of a proton gas. As early as 1944, Wigner and Wilkins ${ }^{8}$ computed $^{9}$ this scattering probability in the case of a hydrogen target. In the particular case of $A=1$, the flux spectrum is the solution to a second-order linear differential

[^124]equation. By assuming that scattering is isotropic in the center of mass, the speed scattering probability $g\left(v \rightarrow v^{\prime}\right)$ is obtained by integrating Eq. (7.8) over $2 \pi$ (Bekurts and Wirtz 1964, p182), without considering the scattering angle, and for scattering from speed $v$ to $v^{\prime}$ :
\[

g\left(\vec{v} \rightarrow \overrightarrow{v^{\prime}}, \vec{V}\right)=\left\{$$
\begin{array}{lll}
0 & \text { si } \quad v^{\prime}<v_{\min }=v_{c d m}-\frac{A}{A+1} v_{r} \\
\frac{2 v^{\prime}}{v_{\max }^{2}-v_{\min }^{2}} & \text { si } & v_{\min } \leq v^{\prime} \leq v_{\max } \\
0 & \text { si } & v^{\prime}>v_{\max }=v_{c d m}+\frac{A}{A+1} v_{r}
\end{array}
$$\right.
\]



Eugène Wigner (left, Public domain) and J. Ernest Wilkins Jr (right, courtesy Wilkins, photograph unknown)

The Maxwell speed distribution of the target atoms is given by:

$$
m(V) d V=4 \pi\left(\frac{m}{2 \pi k T}\right)^{3 / 2} V^{2} e^{-\frac{m V^{2}}{2 k T}} d V
$$

In the chapter on "neutron interaction", the relative speed characterizing the neutron-target collision is given by:

$$
v_{r}^{2}=v^{2}+V^{2}-2 v V \cos \theta
$$

where $\theta$ is the angle between the speeds before collision. If all post-collision directions have equal probabilities, the probability of collision occurring between
angle $\theta$ and $\theta+d \theta$ is equal to $d(\cos \theta) / 2 \equiv d \mu / 2$. The number of collisions per $\mathrm{cm}^{3}$ and per second in this solid angle for a differential element $d V$ of the target velocity for a single neutron is:

$$
d R(\mu, V)=\Sigma_{s} \Phi \frac{d \mu}{2}=N \sigma v_{r} p(V) d V \frac{d \mu}{2} \equiv v N d \sigma\left(v \rightarrow v^{\prime}, V\right)
$$

using the differential element for the differential scattering cross section. The total differential scattering cross section is obtained by integrating over the possible speeds $V$ of the target and for all the incident directions:

$$
\sigma\left(v \rightarrow v^{\prime}\right)=\int_{\mu=-1}^{\mu=+1} d \mu \int_{V=0}^{+\infty} \frac{d \sigma\left(v \rightarrow v^{\prime}, V\right)}{d \mu}=\frac{1}{2 v} \int_{\mu=-1}^{\mu=+1} d \mu \int_{V=0}^{+\infty} v_{r} \sigma_{s} p(V) g\left(v \rightarrow v^{\prime}\right)
$$

Given that $v_{\text {com }}=\frac{\sqrt{v^{2}+A^{2} V^{2}+2 A v \mu}}{A+1}$, after some algebraic calculations, the following equation is finally obtained:

$$
\sigma\left(v \rightarrow v^{\prime}\right)=\sigma_{s} \frac{v^{\prime}}{v^{2}} 9^{2}\left\{\operatorname{erf}\left(\frac{\vartheta v^{\prime}-\varsigma v}{v_{T}}\right) \pm e r f\left(\frac{\vartheta v^{\prime}+\varsigma v}{v_{T}}\right)+e^{\frac{v^{2}-v^{2}}{v_{1 / 2}}}\left[\operatorname{erf}\left(\frac{\vartheta v-\varsigma v^{\prime}}{v_{T}}\right) \mp e r f\left(\frac{\vartheta v+\varsigma v^{\prime}}{v_{T}}\right)\right]\right\}
$$

where $\vartheta \equiv \frac{A+1}{2 \sqrt{A}}, \varsigma \equiv \frac{A-1}{2 \sqrt{A}}, v_{T} \equiv \sqrt{\frac{2 k T}{m_{\text {neurron }}}}$ and the " + " sign implies that $v>v^{\prime}$ while the "-" sign that $v<v^{\prime}$. Expressed in terms of energy, the differential cross section may be written as (Progress in nuclear energy Vol 2 1958, p96):

$$
\begin{aligned}
& \sigma\left(E \rightarrow E^{\prime}\right) \\
& =\sigma_{s} \frac{e^{\frac{E}{k T}}}{E} \frac{\vartheta^{2}}{2}\left\{\begin{array}{l}
e^{-\frac{E^{\prime}}{k T}} \operatorname{erf}\left(\vartheta \sqrt{\frac{E}{k T}}-\varsigma \sqrt{\frac{E^{\prime}}{k T}}\right)+e^{-\frac{E}{k T}} \operatorname{erf}\left(\vartheta \sqrt{\frac{E^{\prime}}{k T}}-\varsigma \sqrt{\frac{E}{k T}}\right) \\
-\left|e^{-\frac{E^{\prime}}{k T}} \operatorname{erf}\left(\vartheta \sqrt{\frac{E}{k T}}+\varsigma \sqrt{\frac{E^{\prime}}{k T}}\right)-e^{-\frac{E}{k T}} \operatorname{erf}\left(\vartheta \sqrt{\frac{E}{k T}}+\varsigma \sqrt{\frac{E^{\prime}}{k T}}\right)\right|
\end{array}\right\}
\end{aligned}
$$

noting carefully that the last two terms in the equation are within absolute values sign. In the case of a proton gas $(A=1)$, the differential scattering cross section, which encompasses the probability of energy transfer, is simplified to (Duderstadt and Hamilton 1976):

$$
\Sigma_{s}\left(E^{\prime} \rightarrow E\right)=\left\{\begin{array}{lll}
\frac{\Sigma_{s}^{H}}{E^{\prime}} \operatorname{erf}\left(\sqrt{\frac{E}{k T}}\right) & E^{\prime}>E & \text { slowing down } \\
\frac{\Sigma_{s}^{H}}{E^{\prime}} \operatorname{erf}\left(\sqrt{\frac{E^{\prime}}{k T}}\right) e^{-\frac{\left(E-E^{\prime}\right)}{k T}} & E^{\prime}<E & \text { upscattering in energy }
\end{array}\right.
$$

In this formula, $\Sigma_{s}^{H}$ is the macroscopic scattering cross section of free hydrogen, which is constant in terms of energy. These formulae may be compared to the pure slowing-down cross section $\quad \Sigma_{s}\left(E^{\prime} \rightarrow E\right)=\Sigma_{s}^{H} /\left[\left(1-\alpha_{H}\right) E^{\prime}\right]=\Sigma_{s}^{H} / E^{\prime} \quad$ since $\alpha_{H}=0$. Defining the reduced speed $x=\sqrt{E /(k T)}$, the total scattering cross section can be computed in terms of energy by integration over the departing energy values $E^{\prime}$, i.e.:

$$
\Sigma_{s}(E)=\frac{\Sigma_{s}^{H}}{\sqrt{\frac{2 E}{m}}} \sqrt{\frac{2 k T}{m}}\left[\left(x+\frac{1}{2 x}\right) \operatorname{erfx} x+\frac{1}{\sqrt{\pi}} e^{-x^{2}}\right]=\frac{\Sigma_{s}^{H}}{x}\left[\left(x+\frac{1}{2 x}\right) \operatorname{erfx}+\frac{1}{\sqrt{\pi}} e^{-x^{2}}\right]
$$

By inserting this scattering cross section and a $1 / v$ absorption term in the thermalization equation, the resulting spectrum is slightly harder compared to a Maxwell distribution. A coarse approximation for a mixture of moderating nuclides consists in substituting $\Sigma_{s}^{H}$ by $\overline{\xi \Sigma_{s}}$ in the formulae. Neglecting the crystal or molecular lattice bonding, as in the free gas model, tends to decrease the slowingdown density, especially near the thermal energy range. Slowing-down is less effective, or in other terms, the target seems heavier, resulting in a decrease in $\xi$ in terms of the number of collisions, and hence a decrease in neutron energy. In the case of zero absorption, this decrease in moderating power increases the migration area, resulting in increased leakage for a finite reactor.

### 7.7 Asymptotic Spectrum

D.S. Selengut in (Yeater 1962, p166; Neutron fluence measurements 1970, p78; Progress in nuclear energy Vol 2 1958, p100)

For an asymptotic flux in a uniform medium far removed from a source of thermal neutrons, the homogeneous balance equation is:

$$
\begin{equation*}
\text { Balance equation: }-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E))+\Sigma_{a} \Phi(\vec{r}, E)=\frac{\partial q}{\partial E} \tag{7.10}
\end{equation*}
$$

where $q$ is the slowing-down density as explained earlier. A classical method to solve this problem consists in expanding the flux by separating the energy and space variables as such (for a plane geometry):

$$
\Phi(\vec{r}, E)=\sum_{n=0}^{+\infty} \phi_{n} \varphi_{n}(E) e^{-\frac{x}{L_{n}}}
$$

The coefficients $\phi_{n}$ must be defined with the boundary conditions at the source. The energy spectrum must verify the eigenvalue equation:

$$
\begin{equation*}
\text { Moment equation: }\left(-\frac{D}{L_{n}^{2}}+\Sigma_{a}\right) \varphi_{n}(E)=\frac{\partial q_{n}}{\partial E} \tag{7.11}
\end{equation*}
$$

where $q_{n}$ is the $n$th order moment obtained by substituting the flux expansion in the definition of the slowing-down density:

> Slowing-down density:
$q(\vec{r}, E) \equiv \int_{0}^{E} d E^{\prime \prime} \int_{E}^{+\infty} d E^{\prime}\left(\Sigma_{S}\left(E^{\prime \prime} \rightarrow E^{\prime}\right) \Phi\left(\vec{r}, E^{\prime \prime}\right) d E^{\prime}-\Sigma_{S}\left(E^{\prime} \rightarrow E^{\prime \prime}\right) \Phi\left(\vec{r}, E^{\prime}\right)\right)$
The smallest eigenvalue, $L_{0}$, represents the asymptotic scattering length, and the associated eigenfunction, the asymptotic spectrum far from the source. The higher modes are of significant importance close to the source only. The next eigenvalue, $L_{1}$, corresponds to re-thermalization of the initial source spectrum, which was not at equilibrium. Historically, a number of attempts have been made to represent the energy spectrum. The first involved expansion of the thermalization kernel of the heavy gas on the eigenfunctions using Laguerre polynomials of order $1, \mathrm{~L}_{\mathrm{n}}(E)$, the latter being a complete basis for polynomials:

$$
\varphi(E) \approx E e^{-\frac{E}{k T_{m}} \sum_{n=0}^{N} \psi_{n} \mathrm{~L}_{\mathrm{n}}(E)}
$$

with $T_{m}$ being the moderator temperature. Precision is improved by increasing the order of the expansion $N$. Another approach consists in expanding the spectrum using a set of Maxwell distributions:

$$
\varphi(E) \approx \sum_{n=0}^{N} \psi_{n} \frac{E}{\left(k T_{n}\right)^{2}} e^{-\frac{E}{k T_{n}}}
$$

given that a spectrum at an intermediate temperature is fairly well represented by a linear combination of two spectra at the extreme temperatures. A third option consists in defining an effective temperature $T_{\text {eff }}$ for which a unique Maxwell distribution is computed:

$$
\varphi(E) \approx \psi \frac{E}{\left(k T_{e f f}\right)^{2}} e^{-\frac{E}{k T_{e f f}}}
$$

This last approach is widely used in industrial calculation codes but there is a drawback in that the effective temperature depends on the absorption in the medium. To quantify a small difference with respect to an equilibrium Maxwell distribution at $T_{0}$ using an effective temperature model such that:

$$
T_{e f f}=T_{0}+\varepsilon T_{0}
$$

and that the perturbation is sufficiently low for $\varepsilon$ to be small enough, the following may be written as a first-order approximation:

$$
\varphi(E)=m\left(k T_{e f f}\right) \approx m\left(k T_{0}\right)+\frac{\partial m(k T)}{\partial T}\left(T_{e f f}-T_{0}\right) \quad \text { with } \quad m(k T) \equiv \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}
$$

to give:

$$
\varphi(E) \approx\left((1-2 \varepsilon)+\frac{E}{k T_{0}} \varepsilon\right) \frac{E}{\left(k T_{0}\right)^{2}} e^{-\frac{E}{k T_{0}}}=\left((1-2 \varepsilon)+\frac{E}{k T_{0}} \varepsilon\right) m\left(k T_{0}\right)
$$

The moment of the cross section with respect to the Maxwell distribution is defined as:

$$
\Sigma_{n} \equiv \int_{0}^{+\infty} m(E)\left(\frac{E}{k T_{0}}\right)^{n} \Sigma(E) d E
$$

In the special case where the cross section varies according to an exponential term $\beta$ in energy $\left(\Sigma(E) \propto E^{\beta}\right)$, the moment can be computed analytically as:

$$
\left\{\begin{aligned}
\Sigma_{0} & =\int_{0}^{+\infty} \frac{E}{\left(k T_{0}\right)^{2}} e^{-\frac{E}{k T_{0}}} C E^{\beta} d E=\int_{0}^{+\infty} C\left(k T_{0}\right)^{\beta} e^{-\frac{E}{k T_{0}}}\left(\frac{E}{k T_{0}}\right)^{\beta+1} d E=C\left(k T_{0}\right)^{\beta} \Gamma(\beta+2) \\
& =\Gamma(\beta+2) \Sigma\left(k T_{0}\right) \\
\Sigma_{n} & =\int_{0}^{+\infty} \frac{E}{\left(k T_{0}\right)^{2}} e^{-\frac{E}{k T_{0}}}\left(\frac{E}{k T_{0}}\right)^{n} C E^{\beta} d E=C\left(k T_{0}\right)^{\beta} \Gamma(n+\beta+2)=\frac{\Gamma(n+\beta+2)}{\Gamma(\beta+2)} \Sigma_{0} \\
& =\Gamma(n+\beta+2) \Sigma\left(k T_{0}\right)
\end{aligned}\right.
$$

By multiplying the slowing-down density [Eq. (7.12)] by $E$ and integrating over all the possible energy values, the rate of energy transfer per unit volume transmitted from the moderator to the neutrons or conversely depending on the thermalization level is:

$$
\int_{0}^{+\infty} E \frac{\partial q}{\partial E} d E=\int_{0}^{+\infty} d E \varphi(E) \int_{0}^{+\infty}\left(E^{\prime}-E\right) \Sigma_{s}\left(E \rightarrow E^{\prime}\right) d E^{\prime} \equiv \int_{0}^{+\infty} \varphi(E) \mu_{1}(E) d E
$$

This equation allows the definition of the first moment for the energy transfer $\mu_{1}(E)$. The global energy transfer rate is computed by averaging this first moment with the flux. Once the calculations have been done, at first order, the following is obtained:

$$
\int_{0}^{+\infty} E \frac{\partial q}{\partial E} d E \approx \frac{1}{2}\left(k T_{0}-k T_{e f f}\right) \frac{1}{\left(k T_{0}\right)^{2}} \int_{0}^{+\infty} d E m_{0}(E) \underbrace{\int_{0}^{+\infty}\left(E^{\prime}-E\right)^{2} \Sigma_{s}\left(E \rightarrow E^{\prime}\right) d E^{\prime}}_{\mu_{2}(E)}
$$

The second moment is the average of the first energy transfer moment by a Maxwell distribution:

$$
m_{2} \equiv \frac{1}{\left(k T_{0}\right)^{2}} \int_{0}^{+\infty} d E m(E) \int_{0}^{+\infty}\left(E^{\prime}-E\right)^{2} \Sigma_{s}\left(E \rightarrow E^{\prime}\right) d E^{\prime}
$$

It depends only on the moderator temperature $T_{0}$. The equations for neutron balance and energy balance are obtained by integrating Eq. (7.10) over energy:

$$
\left\{\begin{array}{l}
\int_{0}^{+\infty}\left[-\frac{D}{L^{2}}+\Sigma_{a}\right] m\left(k T_{e f f}\right) d E=\int_{0}^{+\infty} \frac{\partial q}{\partial E} d E=0 \\
\int_{0}^{+\infty}\left[-\frac{D}{L^{2}}+\Sigma_{a}\right] m\left(k T_{e f f}\right) E d E=\int_{0}^{+\infty} E \frac{\partial q}{\partial E} d E=-\varepsilon k T_{0} \frac{m_{2}}{2}
\end{array}\right.
$$

Using the expansion $m\left(k T_{e f f}\right) \approx\left((1-2 \varepsilon)+\frac{E}{k T_{0}} \varepsilon\right) m\left(k T_{0}\right)$, the moments of the cross sections are inserted:

$$
\left\{\begin{array}{l}
-\frac{(1-2 \varepsilon) D_{0}+\varepsilon D_{1}}{L^{2}}+(1-2 \varepsilon) \Sigma_{a, 0}+\varepsilon \Sigma_{a, 1}=0 \\
-\frac{(1-2 \varepsilon) D_{1}+\varepsilon D_{2}}{L^{2}}+(1-2 \varepsilon) \Sigma_{a, 1}+\varepsilon \Sigma_{a, 2}=-\varepsilon \frac{m_{2}}{2}
\end{array}\right.
$$

The quantities $\varepsilon$ (or $L^{2}$ ) can be removed from this equation system, resulting in a quadratic equation which relates the other averaged quantities to the Maxwell distribution. At first order in $\varepsilon$, the asymptotic scattering length $L_{0}$ can be obtained using:

$$
L_{0}^{2}=\frac{D_{0}}{\Sigma_{a, 0}}\left(1+2\left[\frac{D_{1}}{D_{0}}-\frac{\Sigma_{a, 1}}{\Sigma_{a, 0}}\right]^{2} \frac{\Sigma_{a, 0}}{m_{2}}\right)
$$

It can be seen that $D_{0} / \Sigma_{a, 0}$ is simply the square of the diffusion length computed using neutron constants averaged with a thermal spectrum at $T_{0}$. Expressing $\varepsilon$ as a function of $L^{2}$, the shift in temperature can be obtained:

$$
\frac{T_{e f f}}{T_{0}} \approx 1+2\left[\frac{D_{1}}{D_{0}}-\frac{\Sigma_{a, 1}}{\Sigma_{a, 0}}\right] \frac{\Sigma_{a, 0}}{m_{2}}
$$

This equation can be simplified for the case where $\Sigma_{a}(E) \propto E^{\beta_{a}}$ and $D(E) \propto E^{\beta_{D}}$ :

$$
\frac{T_{e f f}}{T_{0}} \approx 1+2\left[\beta_{D}-\beta_{a}\right] \frac{\Sigma_{a, 0}}{m_{2}}
$$

In the usual case where the diffusion coefficient is constant with energy and where the absorption cross section has a $1 / v\left(\beta_{a}=-1 / 2\right)$ form, we obtain:

$$
\frac{T_{e f f}}{T_{0}} \approx 1+\frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}\left(k T_{0}\right)}{m_{2}}
$$

and, for the heavy gas approximation $(A \gg 1)$, the second moment, which is proportional to the slowing-down power $m_{2}=4 \xi \Sigma_{s}$, may be computed. Hence, the higher the absorption of the medium, the more significant is the correction due to the hardening of the spectrum. For light water reactors, the assumption that the thermal spectrum may be computed using a Maxwell distribution at the moderator temperature leads only to a small error, as will be shown in the next paragraph.

### 7.8 Simplified Solution to Thermalization with Absorption

Theory predicts that in the absence of absorption, thermal neutrons are distributed according to a Maxwell-distributed flux distribution and slowing-down (epithermal) neutrons obey a flux that is inversely proportional to energy. Hence, we may imagine a function linking both asymptotic spectra. In a real absorbing moderator, the solution to the slowing-down equation with an absorption term is a flux spectrum, which deviates from the pure Maxwell distribution. It may be useful to model the flux by a difference function, which measures the deviation from the Maxwell distribution (possibly shifted to the effective temperature as seen earlier), which tends towards an asymptotic $1 / E$ slowing-down spectrum by construction. Assuming that the thermal zone is modeled by a Maxwell distribution despite absorption, the difference function retains its properties as the connecting function between the two asymptotic spectra:


Fig. 7.5 Comparison of a real spectrum with a Maxwell distribution

$$
\Phi(E)=[\underbrace{\frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}}_{m(E)}+\underbrace{\lambda \Delta(E / k T) \cdot \frac{1}{E}}_{\text {Connection function }}] \Phi_{t h}
$$

Figure 7.5 represents a comparison between the spectrum of a $U O X 3.70 \%$ assembly (as calculated by the French spectral code APOLLO2) and the reconstruction of the spectrum with a Maxwell distribution and a $1 / E$ epithermal flux. Visually, it can be found that the reconstruction matches well the calculated flux over a large portion of the spectrum. The fast spectrum has not been modeled, thus explaining the significant difference at high energy. In the thermal energy zone, the real spectrum is slightly harder, i.e. shifted towards higher energies, than the pure Maxwell spectrum due to absorption.

The function $\Delta(E / k T)$ is dimensionless [-] and is globally equal to 0 in the thermalization zone and to 1 in the epithermal zone (Duderstadt and Hamilton 1976, p382; Bekurts and Wirtz 1964, p206). $\lambda$ is a dimensionless normalization coefficient $[-], \Phi_{t h}$ is the level of the thermal neutron flux [neutron $/ \mathrm{cm}^{2} / \mathrm{s}$ ], and $\Phi(E)$ is the flux spectrum [neutron $/ \mathrm{cm}^{2} / \mathrm{s} / \mathrm{eV}$ ]. As we move further from the thermal energy zone, the Maxwell spectrum tends to zero and the junction function $\Delta(E / k T)$ tends to 1 (Fig. 7.6). The value at which the junction function becomes different from 0 (at about 4 for a $P W R$ ) is denoted $\mu$ by C.H. Westcott (Neutron fluence measurements 1970, p48), whose formalism will be detailed later on.

The flux tends towards the epithermal flux which, for a source $Q_{[n . s-1]}$, assuming that slowing-down occurs in a weakly absorbing medium $\Sigma_{a} \ll \xi \Sigma_{s}$, is written as:

Fig. 7.6 Junction function between thermal and epithermal areas for water


$$
\Phi_{\text {epithermal }}(E)=\frac{Q}{\xi \Sigma_{s} E} \approx \frac{\lambda \Phi_{\text {th }}}{E} \text { with }\left(\Delta\left(\frac{E}{k T}\right) \approx 1\right)
$$

i.e.:

$$
Q \approx \lambda \xi \Sigma_{s} \Phi_{t h}
$$

By definition of a medium without leakage, any neutron emitted by the source $Q$ is absorbed between $\left[0, E_{\max }\right]$, with the neutrons being emitted at $E_{\max }$ :

$$
Q=\int_{0}^{E_{\max }} \Sigma_{a}(E) \Phi(E) d E=\int_{0}^{\infty} \Sigma_{a}(E) \Phi(E) d E
$$

with: $\Sigma_{a}(E)$ en $\frac{1}{v}, \quad \Sigma_{a}(E)=\Sigma_{a}(k T) \frac{v_{T}}{v}=\Sigma_{a}(k T) \sqrt{\frac{k T}{E}}$.
where:

$$
\begin{aligned}
Q=\Sigma_{a}(k T) \Phi_{t h} \underbrace{\int_{0}^{\infty} \sqrt{\frac{E}{k T}} \frac{e^{-\frac{E}{k T}} d E}{k T} d E}_{\Gamma(3 / 2)=\sqrt{\pi} / 2}+\underbrace{\lambda \Sigma_{a}(k T) \Phi_{t h} \overbrace{\int_{0}^{\infty} \Delta\left(\frac{E}{k T}\right)\left(\frac{k T}{E}\right)^{3 / 2} \frac{d E}{k T}}^{\approx 1}} & \approx \lambda \Phi_{\text {th }} \Sigma_{a}(k T)
\end{aligned}
$$

Effectively: $\int_{0}^{\infty} \Delta\left(\frac{E}{k T}\right)\left(\frac{k T}{E}\right)^{3 / 2} \frac{d E}{k T}=\int_{0}^{\infty} \Delta(x) \frac{1}{x^{3 / 2}} d x$
With $\Delta(x) \approx 0$ for $x \leq \mu=4$, and $\Delta(x) \approx 1$ for $x \geq \mu=4$ (assuming that $\Delta(x)$ has the shape of a step function that is non-zero towards $x=\mu$ ):

$$
\int_{0}^{\infty} \Delta(x) \frac{1}{x^{3 / 2}} d x \approx\left[-\frac{2}{\sqrt{x}}\right]_{4}^{+\infty}=1
$$

Hence: $\lambda \xi \Sigma_{s} \Phi_{t h}=Q \approx \Sigma_{a}(k T) \frac{\sqrt{\pi}}{2} \Phi_{t h}+\lambda \Sigma_{a}(k T) \Phi_{t h}$
Hence the junction constant: $\lambda \approx \frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}(k T)}{\left(\xi \Sigma_{s}-\Sigma_{a}(k T)\right)}$


This formulation for the flux is only valid under various assumptions employed to obtain this result, especially the fact that absorption must be negligible where there is no leakage and the junction function has a special form. These limitations have led some authors to propose other more precise approaches. In particular, C. H. Westcott proposed a formulation writing the neutron density in the reduced form (with $x=v / v_{T}$ ):

$$
n(x)=\frac{4}{\sqrt{\pi}}\left[(1-b r) x^{2} e^{-x^{2}}+r \frac{\Delta(x)}{x^{2}}\right]
$$

This form inherently includes the Maxwell distribution $m(x)=4 x^{2} e^{-} x^{2} / \sqrt{\pi}$, as well as the junction function meeting the following two conditions:

$$
\lim _{x \rightarrow 0} \frac{\Delta(x)}{x^{2}}=0 \quad \text { and } \quad \lim _{x \rightarrow+\infty} \Delta(x)=1
$$

so that there is a connecting point in the thermal zone and that the flux is of the $1 / E$ shape (neutron density in $1 / x^{2}$ ) in the epithermal zone. Coefficient $b$ satisfies the normalization condition $\int_{0}^{\infty} n(x) d x=1$, i.e.:

$$
b=\frac{4}{\sqrt{\pi}} \int_{0}^{\infty} \frac{1}{x^{2}} \Delta(x) d x
$$

Westcott proposed several empirical cut-off functions $\Delta(x)$ of the form:

$$
\Delta(x)=\left[1+\left(\frac{\mu}{x^{2}}\right)^{m}\right]^{-1} \quad \text { where } m \text { is of order } 7
$$

The Westcott formalism hinges on several hypotheses. Absorption is assumed to be negligible compared to slowing-down in order to compute the $r$ index (i.e. a low value of $r$ ). This is not true, especially if the medium has epithermal absorbers, which is the case for a reactor with uranium 238 in a thermal spectrum. Thus, Westcott was forced to introduce a neutron temperature that is no longer the temperature of the Maxwell spectrum of the moderator, and that deviates even more from the latter when absorption is significant. This temperature is often given by empirical laws such as:
$T=(1+\alpha r) T_{\text {moderator }} \quad$ where $\alpha$ is a parametric coefficient depending on the moderator.
It has no physical meaning other than to shift the thermal Maxwell distribution so as to better fit the true spectrum. Very often, the Westcott model is applied taking $T$ as the moderator temperature. The strength of this model is its relatively simple calculation of the effective cross sections for the reconstruction of the reaction rate. It also relies on the fact that coefficients $g_{(T)}$ and $s_{(T)}$, used to calculate these effective cross sections, depend only on temperature and not on the nature of the moderator (i.e. the same coefficients are obtained for liquid water or solid carbon at a given temperature). A second point is the fact that the medium is assumed to be homogeneous and without leakage (enabling use of the slowing-down model). Once more, depending on the size of the pile, this hypothesis may not be valid. The Westcott model will be discussed in depth later.

### 7.9 Horowitz-Tretiakoff Model

(Neutron fluence measurements 1970, p51)

### 7.9.1 Principle

As early as November 1960, Jules Horowitz ${ }^{10}$ (Photo 7.3) and Oleg Tretiakoff ${ }^{11}$ proposed ${ }^{12}$ a more complex but more precise model that accounts for leakage and heterogeneity. The goal was to eliminate the absorption problem, which empirically modifies the Westcott junction function. In this model, neutron density is written as:

[^125]

A rare historical photograph of an adolescent Jules Horowitz (second row, center) in 1936 during the visit to Metz of the Jewish youth movement Brith Hanoar Hamizra 'hat (Courtesy Horowitz family)

$$
n(x)=m(x)+2 r_{H T} e(x)
$$

with the following normalization: $\int_{0}^{\infty} n(x) d x=1, \int_{0}^{\infty} m(x) d x=\int_{0}^{\infty} \frac{4}{\sqrt{\pi}} x^{2} e^{-x^{2}} d x=1$ and $\int_{0}^{\infty} e(x) d x=0$.
$e(x)$ is a junction function with a zero integral value (Bekurts and Wirtz 1964, p208). The quantity $r_{H T}$ is the Horowitz-Tretiakoff spectrum index, and it will be later seen that it differs from the Westcott spectrum index, hence the $H T$ index which differentiates between them. If it is compared to the slowing-down theory as for the Westcott model, it is found that for large values of $x, n(x) \approx 2 r_{H T}\left(1 / x^{2}\right)$ which is compared to:

$$
n(x)=\frac{Q}{v_{T} \xi \Sigma_{s}} \frac{2}{x^{2}}=\frac{\widehat{\Sigma}_{a} n v_{0}}{v_{T} \xi \Sigma_{s}} \frac{2}{x^{2}}
$$



Photo 7.3 The works of Jules Horowitz (CEA, courtesy Horowitz family)

Thus, the Horowitz-Tretiakoff spectrum index: $r_{H T}=\sqrt{\frac{T_{0}}{T}} \frac{\widehat{\Sigma}_{a}}{\xi \Sigma_{s}}=\sqrt{\frac{4}{\pi} r}$
Coefficients $r$ and $r_{H T}$ are found to differ only by a multiplicative constant (Photo 7.3). For high energies, the Maxwell distribution is almost zero, thus:

$$
e(x) \sim \frac{1}{\mathrm{x}^{2}}
$$

The epithermal junction function $e(x)$ is such that it tends towards $1 / x^{2}$ as $x$ tends towards infinity. For a calculation with two energy groups defined by a cut-off
energy $E_{c}$ corresponding to a speed $v_{c}$ and a reduced speed $x_{c}=v_{c} / v_{T}$, the ratio of speed at $2200 \mathrm{~m} / \mathrm{s}$ to average thermal speed is:

$$
\bar{v}=\int_{0}^{x_{c}} v x n(x) d x
$$

Historically, this ratio is called the UNITA parameter in the CEA code APOLLO1:

$$
U N I T A=\frac{v_{0}}{\bar{v}}=\frac{v_{0}}{v_{T}} \frac{\int_{0}^{x_{c}} n(x) d x}{\int_{0}^{x_{c}} x n(x) d x}=\frac{v_{0}}{v_{T}} \frac{\int_{0}^{x_{c}}\left[m(x)+2 r_{H T} e(x)\right] d x}{\int_{0}^{x_{c}} x\left[m(x)+2 r_{H T} e(x)\right] d x}
$$

For a cut-off (usually used in light water reactors) at $0.625 \mathrm{eV}, x_{c} \approx 3.6$ and $m\left(x_{c}\right) \approx 9 \times 10^{-5}$, meaning that the following approximation on the upper bound of the integral can be made:

$$
\int_{0}^{x_{c}} m(x) d x \approx \int_{0}^{\infty} m(x) d x=1
$$

and also:

$$
\int_{0}^{x_{c}} x m(x) d x \approx \int_{0}^{\infty} x m(x) d x=\frac{2}{\sqrt{\pi}}
$$

These approximations allow calculation of the UNITA parameter:

$$
\text { UNITA }=\frac{v_{0}}{\bar{v}} \approx \sqrt{\frac{T_{0}}{T}} \frac{1+2 r_{H T} \bar{e}}{\frac{2}{\sqrt{\pi}}+2 r_{H T} \overline{x_{e}}}
$$

with: $\bar{e}=\int_{0}^{x_{c}} e(x) d x$ et $\overline{x_{e}}=\int_{0}^{x_{c}} x e(x) d x$.
For a cross section of the $1 / v$ form, the UNITA parameter links the effective cross sections and the average cross sections over the thermal group as follows:

$$
\frac{\widehat{\Sigma}}{\bar{\Sigma}}=\frac{\int_{0}^{v_{c}} \varphi(v) d v}{v_{0} \int_{0}^{v_{c}} n(v) d v}=\frac{\int_{0}^{v_{c}} v n(v) d v}{v_{0} \int_{0}^{v_{c}} n(v) d v}=\frac{\bar{v}}{v_{0}}=\frac{1}{U N I T A}
$$

If the neutron density is a pure Maxwell distribution, the UNITA parameter can be computed analytically as:

$$
\text { UNITA }_{\text {Maxwell }}=\sqrt{\frac{T_{0}}{T}} \frac{\sqrt{\pi}}{2}
$$

For a non-Maxwell distribution,

$$
\bar{e}=\int_{0}^{x_{c}} e(x) d x=\underbrace{\int_{0}^{\infty} e(x) d x}_{0}-\int_{x_{c}}^{\infty} \underbrace{e(x)}_{1 / x^{2}} d x \approx-\frac{1}{x_{c}}=-\frac{v_{T}}{v_{c}}=-\sqrt{\frac{T}{T_{c}}}
$$

To compute $\overline{x_{e}}$, the notion of a reference temperature $T_{r e f}$ is introduced. It corresponds to the temperature at which the reference cross sections are computed and defines a reference reduced speed at the cut-off $x_{c}^{r e f}=v_{c} / v_{T_{r e f}}$ :

$$
\overline{x_{e}}=\int_{0}^{x_{c}} x e(x) d x=\int_{0}^{x_{c}^{\text {ref }}} x e(x) d x+\int_{x_{c}^{\text {ref }}}^{x_{c}} x \underbrace{e(x)}_{\approx 1 / x^{2}} d x
$$

thus:

$$
\overline{x_{e}}={\overline{x_{e}}}^{r e f}-\frac{1}{2} \ln \left(\frac{T}{T_{r e f}}\right)
$$

Calculation of the spectrum index $r_{H T}$ requires evaluation of the slowing-down density at the cut-off. As seen earlier, the asymptotic solution to the slowing-down equation is:

$$
\varphi_{a s}(u)=\frac{q(u)}{\xi \Sigma_{s}(u)}
$$

Similarly, the expressions for flux and neutron density with reduced speed $x=v / v_{T}$ are:

$$
\varphi_{a s}(x)=\frac{2 q(x)}{\xi \Sigma_{s}(x)} \frac{1}{x} \quad n(x)=\frac{\varphi_{a s}(x)}{x v_{T}}=\frac{2 q(x)}{v_{T} \xi \Sigma_{s}(x)} \frac{1}{x^{2}}
$$

The spectrum index $r_{H T}$ (characteristic of the junction between the two domains) is written:

$$
r_{H T}=\frac{q(x)}{v_{T} \xi \Sigma_{s}(x)}
$$

Since any neutron arriving in the thermal domain is eventually absorbed (in the absence of leakage), the slowing-down density is equal to integration over the total absorption:

$$
q(x)=\int_{0}^{x} \Sigma_{a}\left(x^{\prime}\right) \Phi\left(x^{\prime}\right) d x^{\prime}
$$

The flux expression is thus written as follows, using $v=v_{T} x$ and $\Phi(x)=v \quad n(x)$ :

$$
\Phi(x)=v_{T} x m(x)+2 x e(x) \int_{0}^{x} \frac{\Sigma_{a}\left(x^{\prime}\right) x^{\prime} n\left(x^{\prime}\right)}{\xi \Sigma_{s}} d x^{\prime}
$$

To compute the reaction rate, effective cross sections are usually used (this will be discussed further in the chapter on thermalized absorption). These cross sections vary very weakly with the operational conditions and are defined as:

$$
\widehat{\Sigma}_{a}=\frac{\int_{0}^{x_{c}} \Sigma_{a}(x) \Phi(x) d x}{v_{0} \int_{0}^{x_{c}} n(x) d x}=\frac{\int_{0}^{x_{c}} \Sigma_{a}(x) x n(x) d x}{v_{0} \int_{0}^{x_{c}} n(x) d x}
$$

thereby leading to the expression of the slowing-down current in terms of the effective absorption cross section:

$$
q\left(x_{c}\right)=\int_{0}^{x_{c}} \Sigma_{a}(x) \Phi(x) d x=v_{0} \widehat{\Sigma}_{a} \int_{0}^{x_{c}} n(x) d x=v_{0} \widehat{\Sigma}_{a}(1+2 r \bar{e})
$$

At cut-off, the following equations are obtained:

$$
q\left(x_{c}\right)=v_{0} \widehat{\Sigma}_{a}(1+2 r \bar{e})=\xi \Sigma_{s} v_{T} x_{c}^{2} r_{H T} e(x) \quad \text { with : } e\left(x_{c}\right) \sim \frac{1}{x_{c}^{2}}
$$

thus: $r_{H T}=\frac{v_{0} \widehat{\Sigma}_{a}}{\xi \Sigma_{s} v_{T}-2 v_{0} \widehat{\Sigma}_{a} \bar{e}}$
Yet: $v_{0}=\sqrt{\frac{2 k T_{0}}{m}}$ and $v_{T}=\sqrt{\frac{2 k T}{m}}$, hence: $r_{H T}=\frac{\sqrt{\frac{T_{0}}{T}}}{\frac{\xi \Sigma_{s}}{\widehat{\Sigma}_{a}}-2 \sqrt{\frac{T_{0}}{T}} \bar{e}}$
with $\quad \bar{e}=-\sqrt{\frac{T}{T_{c}}}$
resulting finally in the expression of the Horowitz-Tretiakoff spectrum index:

$$
\begin{equation*}
\text { Horowitz-Tretiakoff spectrum index : } r_{H T}=\frac{\sqrt{\frac{T_{0}}{T}}}{\frac{\xi \Sigma_{s}}{\widehat{\Sigma}_{a}}+2 \sqrt{\frac{T_{0}}{T_{c}}}} \tag{7.13}
\end{equation*}
$$

These calculations for two energy groups allow transition from an effective to an average cross section by accounting for moderator temperature variations. In the chapter on neutron feedback, we will describe the full potential value of this approach. The thermalization equation, described previously, introduces the thermalization operator $H$ []:

$$
H[\Phi(E)]=\int_{0}^{\infty} \Sigma_{S}\left(E^{\prime}, E\right) \Phi\left(E^{\prime}\right) d E^{\prime}-\Phi(E) \int_{0}^{\infty} \Sigma_{S}\left(E, E^{\prime}\right) d E^{\prime}
$$

The thermalization equation can thus be written as:

$$
H[\Phi(E)]=\Sigma_{a}(E) \Phi(E)
$$

The thermalization operator is linear and describes the energy transfers between the neutron gas and the moderator. Using the reduced speed $x$ and the neutron lifetime $\ell_{0}$, defined by the formula $\ell_{0}(x)=1 /\left[x \Sigma_{a}(x)\right]$, the slowing-down equation in terms of neutron density is:

$$
\left[H-\frac{1}{\ell_{0}(x)}\right][n(x)]=0
$$

where, thanks to the change invariable $\Sigma_{a}(v) d v=\Sigma_{a}(v(x)) v_{T} x=\Sigma_{a}(x) d x$, the following expression may be deduced: $\ell_{0}(x)=1 /\left[x \Sigma_{a}(x)\right]$. In the case of weak absorption, Horowitz and Tretiakoff use a first-order expansion of $n(x)$ in terms of $r_{H T}$ : $n(x)=m(x)+2 r_{H T} e_{1}(x)$ where $e_{1}(x)$ tends towards $e(x)$ as $x$ tends towards 0 . At first order, the following may be written:

$$
\frac{1}{\bar{\ell}}=\int_{0}^{\infty} \frac{m(x)}{\ell(x)} d x
$$

which is simply the weighting of $1 / \ell(x)$ by a Maxwell distribution. Since $m(x)$ is the solution of the thermalization equation without absorption, $H[m(x)]=0$,

$$
\begin{aligned}
{\left[H-\frac{1}{\ell(x)}\right][n(x)] } & =\left[H-\frac{1}{\ell(x)}\right]\left[m(x)+2 r_{H T} e_{1}(x)\right] \\
& \approx-\frac{m(x)}{\ell(x)}+H\left[2 \sqrt{\frac{T_{0}}{T \xi \Sigma_{s}} \widehat{\Sigma}_{1}(x)}\right]=0
\end{aligned}
$$

thus: $\frac{1}{\xi \Sigma_{s}} H\left[e_{1}(x)\right]=\frac{m(x)}{2 \sqrt{\frac{T_{0}}{T}} \widehat{\Sigma}_{a} \ell(x)}=\frac{\bar{\ell} m(x)}{2 \ell(x)}$ with $\bar{\ell}=\frac{1}{x_{0} \widehat{\Sigma}_{a}}$
It should be noted that use of the weakly-absorbing heavy gas model (Duderstadt and Hamilton 1976, p388) to compute $r_{H T}$ is not inherent to the model, and the calculation may be kept very general, allowing any slowing-down model to be used. The solution to the equation:

$$
\frac{1}{\xi \Sigma_{s}} H\left[e_{1}(x)\right]=\frac{\bar{\ell} m(x)}{2 \ell(x)}
$$

determines the function $e_{1}(x)$, which is characteristic of the moderator and depends solely on temperature. The effective cross section is then given by:

$$
\widehat{\sigma}=\sigma_{0}\left(\bar{m}(T)+2 r_{H T} \bar{e}_{1}(T)\right)
$$

with:
$\begin{cases}\bar{m}(T)=\frac{1}{\sigma_{0} v_{0}} \int_{0}^{\infty} \sigma(x) v m(x) d x & \text { which is a function independent of the moderator } \\ \bar{e}_{1}(T)=\frac{1}{\sigma_{0} v_{0}} \int_{0}^{\infty} \sigma(x) v e_{1}(x) d x & \text { which depends on the moderator }\end{cases}$

### 7.9.2 Case of Absorption Inversely Proportional to Speed

In the case where absorption varies as $1 / v$, the following equations are obtained:
$\left\{\begin{array}{l}r_{H T}=\sqrt{\frac{T_{0}}{T}} \frac{\widehat{\Sigma}_{a}}{\xi \Sigma_{s}}=\frac{v_{0}}{v_{T}} \frac{\widehat{\Sigma}_{a}}{\xi \Sigma_{s}}=\frac{v}{v_{T}} \frac{\Sigma_{a}}{\xi \Sigma_{s}}=\sqrt{\frac{T_{0}}{T}} \frac{\Sigma_{a}{ }^{0}}{\xi \Sigma_{s}}=\frac{\Sigma_{a}(T)}{\xi \Sigma_{s}} \\ \overline{\bar{\ell}}=\int_{0}^{\infty} \frac{m(x)}{\ell(x)} d x=\int_{0}^{\infty} \frac{m(x)}{\frac{1}{x \Sigma_{a}(x)}} d x=\int_{0}^{\infty} \frac{\frac{m(x)}{1}}{x \frac{\Sigma_{a}^{0} x_{0}}{x}} d x=\frac{1}{\ell_{0}} \int_{0}^{\infty} m(x) d x=\frac{1}{\ell_{0}}, \ell(x)=\frac{1}{x \frac{\Sigma_{a}^{0} x_{0}}{x}}=\ell_{0}\end{array}\right.$
where: $\frac{1}{\xi \Sigma_{s}} H\left[e_{1}(x)\right]=\frac{\bar{\ell} m(x)}{2 \ell(x)}=\frac{1}{2} m(x)$

### 7.9.3 Case of a Finite Reactor (with Leakage)

In the case of leakage, neutrons may either be denoted as being absorbed or as leaking from the reactor, i.e.:

$$
\begin{aligned}
Q_{\left[\mathrm{n}: \mathrm{cm}^{3} / \mathrm{s}\right]} & =\int_{0}^{\infty} \Sigma_{a} n v d v+\int_{0}^{\infty} D_{a} B^{2} n v d v=\int_{0}^{\infty} \Sigma_{a} n v d v\left(1+\frac{\int_{0}^{\infty} D_{a} B^{2} n v d v}{\int_{0}^{\infty} \Sigma_{a} n v d v}\right) \\
& =v_{0} \widehat{\Sigma}_{a}\left(1+M^{2} B^{2}\right)
\end{aligned}
$$

where $M^{2}=\int_{0}^{\infty} D_{a} n v d v / \int_{0}^{\infty} \Sigma_{a} n v d v$ is the migration area. The Horowitz-Tretiakoff model is thus corrected using the leakage term:

$$
r_{H T}=\sqrt{\frac{T_{0}}{T}} \frac{\widehat{\Sigma}_{a}}{\xi \Sigma_{s}}\left(1+M^{2} B^{2}\right) \text { and that of Westcott by } r=\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \widehat{\Sigma}_{a} \frac{\Sigma_{s}}{\xi \Sigma_{s}}\left(1+M^{2} B^{2}\right)
$$

### 7.9.4 Thermalization Equation for a Homogeneous Medium

Given that the neutron density is represented in the Horowitz-Tretiakoff model by:

$$
n(x)=m(x)+2 r_{H T} e(x)
$$

the thermalization operator $H$ applied to the neutron density is written as follows, with $P\left(x^{\prime} \rightarrow x\right) n\left(x^{\prime}\right)$ the number of neutrons scattering from the reduced speed $x^{\prime}$ to $x$ :

$$
H[n(x)]=\int_{0}^{\infty} P\left(x^{\prime} \rightarrow x\right) n\left(x^{\prime}\right) d x^{\prime}-n(x) \int_{0}^{\infty} P\left(x \rightarrow x^{\prime}\right) d x^{\prime}
$$

By disregarding the leakage term, the equilibrium condition leads to equating this term to the number of neutrons absorbed:

$$
H[n(x)]=\Sigma_{a}(x) x n(x)
$$

By definition of the Maxwell distribution, i.e. solution to the thermalization equation without absorption, $H[m(x)] \equiv 0$. Further, assuming that absorption is proportional to $1 / v$, the following equation can be written:

$$
\begin{array}{cc}
\Sigma_{a}(x) x=\Sigma_{a}(1) \\
\text { Since : } & r_{H T}=\frac{2}{\sqrt{\pi}} r=\sqrt{\frac{T_{0} \widehat{\Sigma}_{a}}{T \xi \Sigma_{s}}=\frac{\Sigma_{a}(1)}{\xi \Sigma_{s}}}
\end{array}
$$

by substituting $n(x)$ by $m(x)+2 r_{H T} e(x)$ in the slowing-down equation, the equation of the function $e(x)$ is obtained:

$$
\left[\frac{1}{\xi \Sigma_{s}} H-r_{H T}\right][e(x)]=\frac{1}{2} m(x)
$$

Since $r_{H T}$ appears in the operator, the solution $e(x)$ also depends on $r_{H T}$ and since

$$
s(x)=\sqrt{\frac{T}{T_{0}} \int_{0}^{\infty} \frac{\sigma(x)}{\sigma_{0}} e(x) 2 x d x}
$$

so does the function $s(x)$, which minimizes use of the Westcott formalism under the form $\widehat{\sigma}=\sigma_{0}(g+r s)$. It is only in the case of weak capture that $\widehat{\sigma}$ can be assumed as varying linearly with $r$. In the more general case, if the capture term does not have a $1 / v$ shape, the value of $r_{H T}$ is given by:

$$
r_{H T}=\frac{1}{\xi \Sigma_{s}} \int_{0}^{\infty} \Sigma_{a}(x) x n(x) d x
$$

### 7.10 Heavy Gas Model

In certain specific cases, the reduced speed transfer probability $P\left(x^{\prime} \rightarrow x\right)$ may be computed, especially for an elastic collision between a neutron and a target nuclide of mass $A$, as shown in slowing-down theory. The theoretical case of an infinitely heavy $\operatorname{target}\left(A\right.$ tends to infinity) but with a moderating power $\xi \Sigma_{s}$, that is finite at high energy, is called the heavy gas model, and is used to model the behavior of uranium. The thermalization operator degenerates into a differential operator of order two and simplifies as follows [see also, with different notations (Bekurts and Wirtz 1964, p218)]:

$$
H[] \equiv \frac{\xi \Sigma_{s}}{4}\left[x \frac{d^{2}}{d x^{2}}+\left(2 x^{2}-1\right) d x \frac{d}{d x}+4 x\right]
$$

Under this assumption, the function $e(x)$, which is equal to zero when $x=0$, and behaves as $1 / x^{2}$ at infinity, verifies the following differential equation:

$$
x \frac{d^{2} e(x)}{d x^{2}}+\left(2 x^{2}-1\right) \frac{d e(x)}{d x}+4\left(x-r_{H T}\right) e(x)=\frac{8}{\sqrt{\pi}} x^{2} e^{-x^{2}}
$$

The expression for $e(x)$ is hence:
Function $\mathrm{e}(x)$ for a gas of infinite mass: $e(x) \approx \frac{1}{x^{2}}-\frac{2 r_{H T}}{x^{3}}+\frac{2\left(1-r_{H T}^{2}\right)}{x^{4}}+\ldots$
In more realistic complex cases, allowance must be made for the chemical bonding of heavy atoms in an oxide, in a metal, or, for fluids, among molecules. In these cases, the slowing-down calculation cannot be done analytically and only the use of computers can help to resolve the slowing-down operator in a more general situation.

### 7.11 Cadilhac, Horowitz and Soulé Differential Model

In 1962, Cadilhac, ${ }^{13}$ Horowitz and Soulé proposed ${ }^{14}$ [see also (Reactor Physics 1966, volume 1, p311-330)] an extension of the previous model to more general cases where reduced energy, $y$, is used as the independent variable:

[^126]

[^127]$$
y=x^{2}=\frac{E}{k T}
$$

Using this variable, the Maxwell distribution is written as:

$$
m(y)=y e^{-y}
$$

The slowing-down density with up-scattering in energy is given by:

$$
q(y)=\underbrace{\int_{0}^{y} d z^{\prime} \int_{y}^{\infty} \Sigma_{s}\left(z \rightarrow z^{\prime}\right) \Phi(z) d z}_{\text {slowing-down }}
$$

$$
-\underbrace{\int_{y}^{\infty} d z^{\prime} \int_{0}^{y} \Sigma_{s}\left(z \rightarrow z^{\prime}\right) \Phi(z) d z}_{\text {up-scaterering }}
$$

In a medium without leakage, neutrons slowed down under reduced energy $y$ are absorbed (Fig. 7.7):

$$
q(y)=\int_{0}^{y} \Sigma_{a}(z) \Phi(z) d z
$$

The micro-reversibility principle allows definition of the differential scattering cross sections by stipulating that thermal equilibrium is reached when the probability energy gain is the same as that of energy loss (principle derived from statistical mechanics):

$$
\Sigma_{s}\left(y^{\prime} \rightarrow y\right) m\left(y^{\prime}\right)=\Sigma_{s}\left(y \rightarrow y^{\prime}\right) m(y)
$$

It can thus be shown that a solution $q(y)$ exists with the integral form:

Fig. 7.7 Slowing-down density with reduced energy $y$


$$
q(y)=\int_{0}^{\infty} L\left(y, y^{\prime}\right) \frac{d}{d y^{\prime}}\left(\frac{\Phi\left(y^{\prime}\right)}{m\left(y^{\prime}\right)}\right) d y^{\prime}=\int_{0}^{\infty} L\left(y, y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}
$$

with $L\left(y, y,{ }^{\prime}\right)=\int_{0}^{\min \left(y, y^{\prime}\right)} \int_{\max (y, y)}^{\infty} m(z) \Sigma_{s}\left(z \rightarrow z^{\prime}\right) d z d z^{\prime}$ being the solution to the balance equation on $q(y)$. The function $\frac{d}{d y}\left(\frac{\Phi(y)}{m(y)}\right)$ can be interpreted as a deviation function with respect to the equilibrium state, with the deviation being due to absorption. For analytical solutions, we will assume that the scattering differential cross section can be factorized in terms of departure and arrival energies:

$$
\begin{cases}\Sigma_{s}\left(y \rightarrow y^{\prime}\right) m(y)=\alpha(y) \beta\left(y^{\prime}\right) & \text { for } y^{\prime}>y \\ \Sigma_{s}\left(y \rightarrow y^{\prime}\right) m(y)=\alpha\left(y^{\prime}\right) \beta(y) & \text { for } y^{\prime}<y\end{cases}
$$

meaning that the ratio of differential cross sections to reach energy $y_{1}$ or $y_{2}$ does not depend on energy $y$ if $y_{1}$ and $y_{2}$ are greater than $y$. This factorization allows computation of $L\left(y, y^{\prime}\right)$ :

$$
L\left(y, y,{ }^{\prime}\right)=\int_{0}^{\min \left(y, y^{\prime}\right)} \int_{\max \left(y, y^{\prime}\right)}^{\infty} \alpha(z) \beta\left(z^{\prime}\right) d z d z^{\prime}=\underbrace{\int_{0}^{\min \left(y, y^{\prime}\right)} \alpha(z) d z}_{f\left(\min \left(y, y^{\prime},\right)\right)} \cdot \underbrace{\int_{\max \left(y, y^{\prime}\right)}^{\infty} \beta(z) d z}_{s\left(\max \left(y, y,,^{\prime}\right)\right)}
$$

The slowing-down density may thus be calculated by separating the integral into two parts:

$$
\begin{aligned}
q(y) & =\int_{0}^{y} \underbrace{L\left(y, y,{ }^{\prime}\right)}_{f\left(y^{\prime}\right) g(y)} C\left(y^{\prime}\right) d y^{\prime}+\int_{y}^{\infty} \underbrace{L\left(y, y,,^{\prime}\right)}_{f(y) g\left(y^{\prime}\right)} C\left(y^{\prime}\right) d y^{\prime} \\
& =g(y) \int_{0}^{y} f\left(y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}+f(y) \int_{y}^{\infty} g\left(y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}
\end{aligned}
$$

Deriving this integral equation twice leads to a differential equation that can be more easily be treated numerically:

$$
\begin{gathered}
\frac{d q(y)}{d y}=g^{\prime} \int_{0}^{y} f\left(y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}+g(y) f(y) C(y)+f^{\prime} \int_{y}^{\infty} g\left(y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}-f(y) g(y) C(y) \\
\frac{d^{2} q(y)}{d y^{2}}=g^{\prime \prime} \int_{0}^{y} f\left(y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}+\left[g^{\prime} f-f^{\prime} g\right] C(y)+f^{\prime \prime} \int_{y}^{\infty} g\left(y^{\prime}\right) C\left(y^{\prime}\right) d y^{\prime}
\end{gathered}
$$

which can be written as follows:

$$
j(y) q(y)-\frac{d}{d y}\left(k(y) \frac{d q(y)}{d y}\right)=C(y)
$$

with:

$$
\left\{\begin{array}{l}
j(y)=\frac{1}{f} \frac{d}{d y}\left(\frac{f^{\prime}}{m(y) \Sigma_{s}(y)}\right)=\frac{1}{g} \frac{d}{d y}\left(\frac{g^{\prime}}{m(y) \Sigma_{s}(y)}\right) \\
k(y)=\frac{1}{f^{\prime} g-f g^{\prime}}=\frac{1}{m(y) \Sigma_{s}(y)}
\end{array}\right.
$$

The Cadilhac operator $J[q(y)] \equiv\left\{j(y)-\frac{d}{d y}\left(k(y) \frac{d}{d y}\right)\right\}[q(y)]$ is a Hermitian operator that is positive definite and becomes a second-order differential operator in the Cadilhac model. Historically, this model was dubbed the Cadilhac secondary model. This operator is exact for a gas of monatomic hydrogen and for a free gas of heavy atoms. Furthermore, it is a good approximation for all common moderators [P. R. Haubert and N. R. Meyvaert in (Reactor Physics 1966, volume 1, p334)].

Given that:

$$
\begin{aligned}
f^{\prime} g-f g^{\prime} & =\alpha(y) \int_{y}^{\infty} \beta\left(y^{\prime}\right) d y^{\prime}+\beta(y) \int_{0}^{y} \alpha\left(y^{\prime}\right) d y^{\prime}=\int_{0}^{\infty} m(y) \Sigma_{s}\left(y \rightarrow y^{\prime}\right) d y^{\prime} \\
& =m(y) \Sigma_{s}(y)
\end{aligned}
$$

the following functions are of more practical use:

$$
F(y)=\Sigma_{s}(\infty) y e^{-y} k(y) \quad \text { and } \quad G(y)=\xi \Sigma_{s}(\infty) y^{2} e^{-y} j(y)
$$

and are set up as follows:

$$
\lim _{y \rightarrow \infty} F(y)=1 \quad \text { and } \quad \lim _{y \rightarrow \infty} G(y)=1
$$

Assuming that, for the particular case where $\alpha(y)=\beta(y)$, which is equivalent to the fact that the energy distribution after collision does not depend on the energy before, i.e. the neutron is not aware of its history, then $j(y)=0$. This is the case for an ideal moderator, characterized only by $F(y)=\Sigma_{s}(\infty) y e^{-y} k(y)=\Sigma_{s}(\infty) / \Sigma_{s}(y)$. Conversely, where $\xi \Sigma_{s}$ remains finite, a collision changes the energy distribution and an infinite number of collisions is required to thermalize the neutrons, hence, $k$ $(y)=0$ and $\Sigma_{s}$ is infinite. Furthermore, if $G(y)=1$, the infinitely heavy gas model is obtained. The Cadilhac, Horowitz and Soulé differential model is thus an intermediate between the ideal moderator and a heavy gas, and leads to these two extreme cases. For example, the slowing-down functions for hydrogen $(A=1)$, whose slowing-down differential cross section verifies the factorizing principle for $y$ and $y^{\prime}$, are written as:

$$
\left\{\begin{array}{l}
\frac{1}{F(y)}=\left(1+\frac{1}{2 y}\right) \operatorname{erf} \sqrt{y}+\frac{e^{-y}}{\sqrt{\pi y}} \\
G(y)=F(y)-y \frac{d F(y)}{d y}=\left(\operatorname{erf} \sqrt{y}+\frac{e^{-y}}{\sqrt{\pi y}}\right) F^{2}(y)
\end{array}\right.
$$

The model transforms the computation of a thermalized spectrum to solving a second-order differential equation. This resolution became one of the first applications of computers to neutron physics in the Department of Applied Mathematics at Saclay (Reuss 2007, p60). Cadilhac's differential secondary model of thermalization, besides being one of the most advanced models, starts with the neutron balance with the reduced speed $x$ :

$$
S(x)+H[n(x)]=n(x) x\left(\Sigma_{a}(x)+D(x) B^{2}\right)
$$

The term on the left corresponds to the sources (fission) and to slowing-down (H [ $n(x)$ ] operator), the second term corresponds to the sum of the absorptions and leakage. The equation to be solved is hence (Fuel burn-up predictions 1968, p37):

$$
\frac{1}{4} \frac{d}{d x} \frac{1}{G(x)}\left(x \frac{d y}{d x}+2\left(x^{2}-1\right) y\right)=x \Sigma(x) n_{m}(x)
$$

with $y(x)=(1+\Sigma(x) H(x)) n_{m}(x), \Sigma(x)=\frac{V_{c} \Sigma_{a, c}(x)}{V_{m} \xi \Sigma_{s}} \frac{n_{c}(x)}{n_{m}(x)}+\frac{\Sigma_{a, m}(x)}{\xi \Sigma_{s}}+\frac{D(x) B^{2}}{\xi \Sigma_{s}}$.
$n_{c}(x)\left(\right.$ resp. $\left.n_{m}(x)\right)$ is the mean density of neutrons in the fuel (respectively in the moderator). Their ratio can be computed using the theory developed by Amouyal-Benoist-Horowitz, which will be described in greater detail in Chap. 14. The functions $G(x)$ and $H(x)$ describe the thermalizing medium and are adjusted once and for all, to account for bonding energy, both interatomic and intermolecular. Several models are available: the Egelstaff model for graphite, the Nelkin model for light water, and the Butler model for heavy water.

### 7.12 Application of the Cadilhac Model to Heterogeneous Media

Extension of the Cadilhac model to heterogeneous cells was first proposed in 1966 by Jean-Pierre de Brion ${ }^{15}$. At that time, the heterogeneous cell to which the model was to be applied was the French UNGG reactor, which was the CEA reference at that time.

[^128]The slowing-down density, $q$, is related to the non-equilibrium function $C$ through the secondary thermalization operator $J$, given by the following formula:

$$
\begin{aligned}
C(y) \equiv \frac{d}{d y}\left(\frac{\Phi(y)}{m(y)}\right) \quad J[q(y)] & \equiv\left\{j(y)-\frac{d}{d y}\left(k(y) \frac{d}{d y}\right)\right\}[q(y)] \\
C & =J[q]
\end{aligned}
$$

Using these notations, the thermalization equation in a finite medium, and in the framework of the diffusion approximation (which will be explored later), is written as:

$$
C(y)=J\left[\int_{z=0}^{z=y}\left(-D \Delta \Phi(r, z)+\Sigma_{a}(z) \Phi(r, z)\right) d z\right]=\left\{j(y)-\frac{d}{d y}\left(k(y) \frac{d}{d y}\right)\right\}[q(y)]
$$

The Fermi asymptotic form of the flux generated by a source $S$ is written as:

$$
\Phi(y)=\frac{S}{\xi \Sigma_{s} y}
$$

de Masfrand, with whom he had three children. He defended a higher doctorate in May 1973. He then left reactor physics for particle physics, in which he pursued an international career. After 2 years at Rochester in the United States, then at Brookhaven National Laboratory on Long Island, he joined CERN with Carlo Rubbia, and published several papers in the field of particle physics. Around 1985, he left particle physics and joined the Direction of Military Applications at Bruyères le Châtel for a more confidential career at BIII/PTN Service (work on the ELSA electron accelerator), before retiring in 1997. He died on August 18, 1998.

(Courtesy De Brion family)

If the thermalization model were true, the following would be obtained:

$$
k(y)=\frac{1}{\Sigma_{s}(y) m(y)}
$$

When reduced energy $y$ tends to infinity, it may be approximated by:

$$
C(y)=J[q] \approx S j(y)
$$

Thus leading to the equation $j(y)$ :

$$
j(y) \underset{y \rightarrow+\infty}{\approx} \frac{e^{y}}{\xi \Sigma_{s} y^{2}}
$$

The following equations are obtained by accounting for the asymptotic nature of functions $j(y)$ and $k(y)$, and by introducing the reduced speed:

$$
\left\{\begin{array}{l}
j(y)=\frac{e^{y}}{\xi \Sigma_{s} y^{2}} G(x) \\
k(y)=\frac{e^{y}}{\xi \Sigma_{s} y} H(x)
\end{array} \quad y=x^{2}\right.
$$

Instead of using the flux $\Phi(y)$, the neutron density $n(x)$ is used, since $\int_{y=0}^{y=+\infty} \Phi(y)$ $d y$ is a divergent integral, which is not the case of $\int_{x=0}^{x=+\infty} n(x) d x$. Since $y=x^{2}$, and $\Phi(y) d y=x n(x) d x$, then $\Phi(y)=n(x) / 2$.

The thermalization equation in a finite medium is written as $F(y)=\Sigma_{s}(\infty) x^{2}$ $e^{-x^{2}} k(x)$ as defined in the previous paragraph:

Thermalization equation expressed in terms of neutron density:

$$
\begin{equation*}
\frac{d\left(1+F(x) \frac{-D \Delta+\Sigma_{a}(x)}{\xi \Sigma_{s}}\right)}{d x}\left[\frac{n(x)}{x^{2} e^{-x^{2}}}\right]=\frac{4 G(x)}{\xi \Sigma_{s} x^{3} e^{-x^{2}}} \int_{z=0}^{z=x}\left(-D \Delta+\Sigma_{a}(z)\right)[z n(z)] d z \tag{7.15}
\end{equation*}
$$

Hence, the thermalization equation can be written as the second-order homogeneous differential equation for the speed and space variables. Thus, two boundary conditions on the speed and two others on space are required to define a completely new solution. At the origin of speeds, the slowing-down density must be zero.

$$
\left\{\begin{array}{l}
q(x)=\int_{z=0}^{z=x}\left(-D \Delta+\Sigma_{a}(z)\right)[z n(z)] d z \\
n(r, x) \approx \frac{1}{2} \frac{d^{2} n(r, 0)}{d x^{2}} x^{2}
\end{array}\right.
$$

In this case, the equations can be integrated with respect to the reduced energy:

$$
\begin{aligned}
& \left(1+F(x) \frac{-D \Delta+\Sigma_{a}(x)}{\xi \Sigma_{s}}\right)[n(r, x)] \\
& -\frac{1}{2} x^{2} e^{-x^{2}} \frac{d^{2} n(r, 0)}{d x^{2}}=\frac{4 x^{2} e^{-x^{2}}}{\xi \Sigma_{s} x^{3} e^{-x^{2}}} \int_{x^{\prime}=0}^{x^{\prime}=x} \frac{G\left(x^{\prime}\right)}{x^{\prime 3} e^{-x^{\prime 2}}} q\left(x^{\prime}\right) d x^{\prime}
\end{aligned}
$$

As for the boundary condition at infinity, the Fermi asymptotic flux model may be used (it may also be rendered more complex using the Greuling-Goertzel model):

$$
\Phi(y)=\frac{S}{\xi \Sigma_{s} y} \quad \text { hence }: n(x)=\frac{2 S}{\xi \Sigma_{s} x^{2}}
$$

The dominant term for the neutron density population in the epithermal range thus varies as $1 / x^{2}$.

As for the spatial aspects, we will consider a cell comprising a fuel cylinder of radius $a$, surrounded by a cylinder of moderator of external radius $b$. In a multi-cell approach where a cell is repeated radially to form a lattice, symmetric boundary conditions for the flux at the edges may be applied. At the fuel/moderator interface, an extrapolation length is used that is inverse to the logarithmic derivative of the flux $\lambda=\Phi(a) / \Phi^{\prime}(a)$. J. P. de Brion expressed flux in a cell as the superposition of two fluxes. The first flux $\Phi_{1}(r)$ is the source in the cell while assuming that the fuel rod is a black body for neutrons (absorption of the infinite rod, i.e. that no neutrons entering the rod can escape). $\Phi_{2}(r)$ corresponds to the neutron current entering the moderator.


The fluxes in these groups satisfy the following equations:

$$
\left\{\begin{array}{l}
-D \Delta \Phi_{1}(r, x)=S(x) \quad \text { with }\left(\frac{\partial \Phi_{1}(r, x)}{\partial r}\right)_{b}=0 \\
\Delta \Phi_{2}(r)=0 \quad \text { with } \Phi_{2}(a)=4 J_{+}(a)=4\left(1-P_{S V}\right) J_{-}(a)
\end{array}\right.
$$

$S(x)$ is taken as the source of neutrons from the black-body radiation problem and is independent of $r . P_{S V}$ is the probability that a neutron entering the fuel in a uniform and isotropic fashion via its surface $S$ will be captured in volume $V$ of the fuel (here, the same notations are used as in Chap. 8).

Integration of the system of differential equations leads to:

$$
\left\{\begin{array}{l}
\Phi_{1}(r, x)=-\frac{S(x)}{4}\left(r^{2}-a^{2}\right)+\frac{S(x)}{2} b^{2} \ln \frac{r}{a}+\lambda_{\text {blackbody }}\left(\frac{S(x)}{2}\left(\frac{b^{2}}{a}-a\right)\right) \\
\Phi_{2}(x)=\frac{4\left(1-P_{S V}\right)}{P_{S V}} \frac{D}{\lambda} \Phi(a, x) \text { to the extent that } P_{S c} J_{-}(a)=S\left(\frac{\partial \Phi(r, x)}{\partial r}\right)_{a}=D \frac{\Phi(a, x)}{\lambda}
\end{array}\right.
$$

The first equation is the well-known solution to the Milne problem, which will be discussed in the chapter on the transport equation. The second equation leads to a spatially flat flux in the moderator. Since the true flux has the same shape as $\Phi_{1}(r, x)$, using the extrapolated length from the real problem, the following equations are obtained:

$$
\begin{aligned}
\Phi(r, x) & =-\frac{S(x)}{4}\left(r^{2}-a^{2}\right)+\frac{S(x)}{2} b^{2} \ln \frac{r}{a}+\lambda_{\text {blackbody }}\left(\frac{S(x)}{2}\left(\frac{b^{2}}{a}-a\right)\right) \\
& =\Phi_{1}(r, x)+\Phi_{2}(x)
\end{aligned}
$$

In the particular case of $r=a$, this equation is written as:

$$
\begin{aligned}
\Phi(a, x) & =\lambda\left(\frac{S(x) b^{2}}{2 a}-\frac{S(x) a}{2}\right) \\
& =\lambda_{\text {blackbody }}\left(\frac{S(x)}{2}\left(\frac{b^{2}}{a}-a\right)\right)+\frac{4\left(1-P_{S V}\right)}{P_{S V}} \frac{D}{\lambda} \Phi(a, x)
\end{aligned}
$$

from which the following may be deduced:

$$
\lambda=\lambda_{\text {black body }}+\frac{4\left(1-P_{S V}\right)}{P_{S V}} D
$$

Several authors since Chandrasekhar have studied the behavior of $\lambda_{\text {black body }}$. The following expression is obtained from the literature (in units of mean free path $1 / \Sigma_{t}$ ):

$$
\lambda_{\text {black body }} \approx \frac{0.7104 \Sigma_{t} a+0.545}{\Sigma_{t} a+0.409}
$$

When radius $a$ tends towards infinity, the limit to the slab problem is obtained, i.e. 0.7104 . When the radius tends towards 0 , since $J_{-}=D \Phi^{\prime} \rightarrow \Phi / 4$ and $D=1 /\left(3 \Sigma_{t}\right)$ in the diffusion approximation, the following expressions are obtained:
$\lambda_{\text {blackbody }[\mathrm{cm}]}=\frac{\Phi}{\Phi^{\prime}} \underset{a \rightarrow 0}{=} \frac{4}{3 \Sigma_{t}}$ hence $\lambda_{\text {blackbody }}=\frac{4}{a \rightarrow 0} \frac{4}{3} \approx \frac{0.545}{0.409}$ in units of mean free path
The capture probability in the cylindrical rod is related to the leakage probability without collision in this same rod by the reciprocity theorem for collision probabilities, with the mean chord $\langle R\rangle$; its calculation will be discussed in detail in Chap. 8:

$$
P_{S V}=\langle R\rangle \Sigma_{t} P_{V S}=2 a \Sigma_{t} P_{V S}
$$

The leakage probability without collision $P_{V S, 0}$ for a cylinder includes the Bessel functions. It is given by (Duderstadt and Martin 1979):

$$
P_{V S, 0}=\frac{2 \Sigma_{t} R}{3}\binom{2\left[\Sigma_{t} R K_{1}\left(\Sigma_{t} R\right) I_{1}\left(\Sigma_{t} R\right)+K_{0}\left(\Sigma_{t} R\right) I_{0}\left(\Sigma_{t} R\right)-1\right]}{+K_{1}\left(\Sigma_{t} R\right) I_{0}\left(\Sigma_{t} R\right)-K_{0}\left(\Sigma_{t} R\right) I_{1}\left(\Sigma_{t} R\right)+\frac{K_{1}\left(\Sigma_{t} R\right) I_{1}\left(\Sigma_{t} R\right)}{\Sigma_{t} R}}
$$

The leakage probability with multiple collisions $P_{V S}$ can be computed as a function of $P_{V S, 0}$ using a method that will be described in Chap. 8.

The numerical resolution of Eq. (7.15) can be carried out by projecting the neutron density on a basis of orthogonal eigenfunctions of the Laplace operator in cylindrical geometry (Bessel functions). This mathematical shortcut eliminates the space variable in the equations and helps to deal with the Laplace operator in the differential equation. The boundary conditions of the problem (in space and energy) are those seen earlier.

This example of the heterogeneous treatment for two media shows that it is possible using the secondary thermalization model to deal with more complex problems than the infinite lattice problem by adopting ingenious techniques. Moreover, the problem can be extended to several zones at the cost of introducing balance equations on neutron densities, in media coupled by collision probabilities.

### 7.13 Graphical Representation of Flux over the Energy Spectrum

Obtaining the shape of the flux spectrum in the thermal and epithermal domains was described earlier. In the fast zone, the fission spectrum is the dominant term, and can be described for instance by the formalism proposed by Watt (Neutron fluence measurements 1970, p141):


Fig. 7.8 Plot of $\int_{E_{g}}^{E_{g-1}} \Phi(E) d E=f\left(E_{g}\right)$ for $3.7 \%$ fuel at $42,500 \mathrm{MWd} /$ ton

$$
\Phi_{\text {fast }}(E)=n_{\text {fast }} \sqrt{E} e^{-\frac{E}{E_{0}}} \sqrt{\frac{2 E}{m}}
$$

This fast neutron shape is added to the previous spectrum using a new junction function. In the end, the flux spectrum in terms of energy may be plotted (Fig. 7.8) using a classical representation with $E \Phi(E)$ on the ordinates axis, as a function of a logarithmic scale with decreasing energy (i.e. increasing lethargy).

### 7.14 True Moderators

(Neutron fluence measurements 1970, p24)
In the case of a true moderator (e.g. water), the thermal spectrum is shifted to the close epithermal range due to absorption (an effect known as a "spectrum hardening"). For a moderator of infinite size, this hardening can be approximated using a "neutron" temperature that is higher than the temperature of the moderator which depends on the slowing-down power $\xi \Sigma_{s}{ }^{16}$.

[^129]Table 7.3 Some values of the neutron temperature coefficient

| Moderator | $a$ |
| :--- | :--- |
| Light water | 5.3 |
| Heavy water | 5.4 |
| Graphite | 7.4 |

$$
\underbrace{T_{\text {neutronic }}}=T\left(1+a \frac{\Sigma_{a}(k T)}{\xi \Sigma_{s}}\right)
$$

## Neutron effective <br> temperature

see (Table 7.3) for values of $a$.
For a moderator of finite size and with leakage $D B^{2}$ (Barjon 1993, p247), from De Sobrino and Clark, gives the following equation [also in (Bekurts and Wirtz 1964, p210)]:

$$
T=T_{0}\left(1+0.73 \quad A \frac{\Sigma_{a}\left(k T_{0}\right)}{\Sigma_{s}}+0.70 A \frac{D B^{2}}{\Sigma_{s}}\right)
$$

This formula implies that the spectrum becomes harder as leakage increases. It is valid not only for positive leakage, but also when the leakage balance is negative (neutrons are introduced into the core, i.e. $B^{2}<0$ ).


In the literature ${ }^{17}$, the following is also found:

$$
T=T_{0}\left(1+0.45 \quad \frac{2 A \Sigma_{a}(E) \sqrt{\frac{E}{k T_{0}}}}{\Sigma_{s}}\right)=T_{0}\left(1+0.90 A \frac{\Sigma_{a}\left(k T_{0}\right)}{\Sigma_{s}}\right)
$$

### 7.15 Heating and Cooling by Scattering

Let us consider the thermalization equation in the permanent state for a scattering and absorbing medium:

$$
-D(E) \Delta \Phi(\vec{r}, E)+\Sigma_{t}(E) \Phi(\vec{r}, E)=\int_{E^{\prime}=0}^{E^{\prime}=+\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}
$$

Supposing that the flux is expressed in a factorized form with a space-dependent function and an energy-dependent function $\Phi(\vec{r}, E)=\phi(E) \varphi(\vec{r})$ where $\phi(E)$ is a spectrum normalized to one. This equation is expressed in energy density using the quantity $E n(\vec{r}, E)=E \Phi(\vec{r}, E) / v$ by multiplying the previous equation by the energy and then integrating with respect to $E$ :

$$
\begin{aligned}
& \int_{E=0}^{E=+\infty}\left(-E D(E) \Delta \Phi(\vec{r}, E)+E \Sigma_{t}(E) \Phi(\vec{r}, E)\right) d E \\
& \quad=\int_{E=0}^{E=+\infty} d E E \int_{E^{\prime}=0}^{E^{\prime}=+\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}
\end{aligned}
$$

By substituting the total collision rate by an absorption and scattering term $\Sigma_{t}(E)=\Sigma_{a}(E)+\Sigma_{s}(E)$ and noting that $\Sigma_{s}(E)=\int_{E^{\prime}=0}^{E^{\prime}=+\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) d E^{\prime}$, this equation may be re-written as follows (Bekurts and Wirtz 1964, p213):

$$
-\bar{E}_{D} \bar{D} \Delta \varphi(\vec{r})+\bar{E}_{\Sigma_{a}} \overline{\Sigma_{a}} \varphi(\vec{r})=\varphi(\vec{r}) \int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty}\left[E-E^{\prime}\right] \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(E^{\prime}\right) d E^{\prime}
$$

where $\bar{E}_{D}$ is the mean energy weighted by the diffusion coefficient and $\bar{E}_{\Sigma_{a}}$ is the energy weighted by the absorption cross section:

[^130]\[

$$
\begin{aligned}
\bar{E}_{D} \equiv \frac{\int_{E=0}^{E=+\infty} E D(E) \varphi(E) d E}{E=+\infty} D(E) \varphi(E) d E & \text { and } \bar{E}_{\Sigma_{a}} \equiv \frac{\int_{E=0}^{E=+\infty} E \Sigma_{a}(E) \varphi(E) d E}{\int_{E=0}^{E=+\infty} \Sigma_{a}(E) \varphi(E) d E} \\
\bar{D} \equiv \frac{\int_{E=0}^{E=+\infty} D(E) \varphi(E) d E}{\int_{E=+\infty}^{E=+\infty}} \varphi(E) d E & \text { and } \\
\Sigma_{a} & \equiv \frac{\int_{E=0}^{E=+\infty} \Sigma_{a}(E) \varphi(E) d E}{\int_{E=0}^{E} \varphi(E) d E}
\end{aligned}
$$
\]

Assuming that absorption is inversely proportional to speed, by definition, $\bar{E}_{\Sigma_{a}}=\bar{E}=3 \mathrm{kT} / 2$. Integrating the thermalization equation directly with respect to energy (without first multiplying by $E$ as done previously), the following balance equation is obtained:

$$
\begin{aligned}
& \int_{E=0}^{E=+\infty}-D(E) \Delta \Phi(\vec{r}, E) d E+\int_{E=0}^{E=+\infty} \Sigma_{t}(E) \Phi(\vec{r}, E) d E \\
& =\int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}=\int_{E=0}^{E=+\infty} \Sigma_{s}(E) \Phi(\vec{r}, E) d E
\end{aligned}
$$

which simplifies to: $-\bar{D} \Delta \varphi(\vec{r})+\overline{\Sigma_{a}} \varphi(\vec{r})=0$.
By combining this equation with the balance equation on energy to eliminate $\overline{\Sigma_{a}} \varphi(\vec{r})$, the integrated thermalization equation may be obtained in the form:

Scattering heating/cooling equation:

$$
\begin{equation*}
\bar{D}\left(\bar{E}-\bar{E}_{D}\right) \frac{\Delta \phi(\vec{r})}{\phi(\vec{r})}=\int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty}\left(E-E^{\prime}\right) \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \varphi\left(E^{\prime}\right) d E^{\prime} \tag{7.16}
\end{equation*}
$$

Since $\bar{E}_{D}$ cannot be equal to $\bar{E}$ (otherwise the diffusion coefficient would be proportional to $1 / v!$ ), the sign of the double integral term depends on the LHS term. If the spatial shape of the flux verifies $\Delta \varphi(\vec{r}) / \varphi(\vec{r})=0$, i.e. in the absence of spatial scattering, the RHS term becomes zero if the spectrum is equal to a Maxwell distribution that leads to perfect equilibrium. Otherwise, depending on the sign of the LHS term, a given volume would gain or lose energy owing to scattering collisions. This is called heating or cooling by scattering and may be measured by inserting a neutron pulse into a non-multiplying medium so as to characterize its properties. For instance, the effect due to a small temperature variation close to a reference temperature $T_{0}$ may be quantified this way. Differentiation of $\bar{D}$ with respect to $T$ leads to:

$$
\frac{d \bar{D}}{d T}=\frac{d\left(\int_{E=0}^{E=+\infty} D(E) \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}} d E\right)}{d T}=-\frac{2 \bar{D}}{T}+\frac{\bar{E}_{D} \bar{D}}{k T^{2}}
$$

where :

$$
\bar{E}_{D}=2 k T+k T^{2} \frac{d \ln \bar{D}}{d T}
$$

based on the fact that $d \log \bar{D}=d \bar{D} / \bar{D}$. A first-order Taylor expansion of the Maxwell distribution with respect to temperature leads to:

$$
\phi(E)=\frac{E}{(k T)^{2}} e^{-\frac{E}{k T}} \approx \underbrace{\frac{E}{\left(k T_{0}\right)^{2}} e^{-\frac{E}{k T_{0}}}}_{m T_{0}(E)}\left(1+\frac{T-T_{0}}{T_{0}}\left(\frac{E}{k T_{0}}-2\right)\right)
$$

By inserting this equation in the double thermalization integral, the following equation is reached:

$$
\begin{aligned}
& \int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty}\left[E-E^{\prime}\right] \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(E^{\prime}\right) d E^{\prime} \\
& \quad \approx \frac{T-T_{0}}{T_{0}} \int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty} E^{\prime}\left[E-E^{\prime}\right] \Sigma_{s}\left(E^{\prime} \rightarrow E\right) m_{T_{0}}\left(E^{\prime}\right) d E^{\prime}
\end{aligned}
$$

noting that the double integral applied to a Maxwell distribution gives zero (perfect equilibrium state), the second-order moment, denoted $m_{2}$, is defined as:

$$
\begin{aligned}
m_{2} & \equiv \frac{1}{\left(k T_{0}\right)^{2}} \int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty}\left[E-E^{\prime}\right]^{2} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) m_{T_{0}}\left(E^{\prime}\right) d E^{\prime} \\
& =\frac{2}{\left(k T_{0}\right)^{2}} \int_{E=0}^{E=+\infty} d E \int_{E^{\prime}=0}^{E^{\prime}=+\infty} E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) m_{T_{0}}\left(E^{\prime}\right) d E^{\prime}
\end{aligned}
$$

These results are introduced into Eq. (7.15) and using $\bar{E}=3 k T / 2$ and $d \ln T=d T / T$, finally, we obtain:

$$
\bar{D} \frac{\Delta \phi(\vec{r})}{\phi(\vec{r})} \frac{k T}{2}\left(1+2 \frac{d \ln \bar{D}}{d \ln T}\right)=\frac{1}{2} k\left(T-T_{0}\right) m_{2}
$$

Supposing that the spatial flux follows an attenuation law (this will be discussed further in the section on diffusion theory):

$$
\Delta \phi(\vec{r})-\frac{1}{M^{2}} \phi(\vec{r})=0
$$

Where $M^{2}=\bar{D} / \overline{\Sigma_{a}}$ is the migration area. The previous equation is then inserted in the heating/cooling equation, and assuming that $T \approx T_{0}$ in the LHS term:

$$
\frac{T-T_{0}}{T_{0}} \approx \overline{\Sigma_{a}}\left(\frac{1+2 \frac{d \ln \bar{D}}{d \ln T}}{m_{2}}\right)
$$

Given that the diffusion coefficient increases experimentally with temperature (e.g. in water, decreasing the density allows neutrons to scatter further), it may be seen that heating occurs when more neutrons are brought in a given volume by scattering than are lost through absorption. This conclusion holds true only for non-multiplying moderators. For a multiplicating medium where $\Delta \phi(\vec{r}) / \phi(\vec{r})<0$, no conclusions should be drawn concerning the subsequent cooling of the medium.

### 7.16 Thermalized Absorption

(Neutron fluence measurements 1970, p48)
The problem of calculating absorption in a thermalized spectrum was outlined at the very start of thermal piles, whether the moderator was of graphite-as in the case of Fermi's pile-or in experimental reactors with heavy or light water, as with the Hanford pile. The need to compute fuel depletion using the Bateman equation implies a good knowledge of the absorption and fission cross sections of the main fuel nuclides. Further, calculation of the activation of a detector or of the absorption of a cadmium sheet requires knowledge of the cross section in the spectrum considered. C. H. Westcott ${ }^{18}$ of Atomic Energy of Canada Ltd (Chalk River, Ontario, Canada) proposed a formalism in the 1950s to characterize thermal spectra.

He suggested a simple method to compute the absorption of nuclides by calculating an "effective" cross section in a thermal spectrum using basic data (cross

[^131]section at $2200 \mathrm{~m} / \mathrm{s}$ and the excess resonance integral). This technique, called the Westcott formalism, is used in codes for fuel cycles that do not have a refined neutron spectrum calculation to condense multi-group cross sections. The initial Westcott model provided coefficients $g_{(T)}$ and $s_{(T)}$ for some nuclides, and these were pre-computed in terms of temperature $T$ of the neutron spectrum:
\[

$$
\begin{equation*}
\text { Westcott model : } \sigma_{\text {effective }}=\sigma_{0}\left(g_{(T)}+r \cdot s_{(T)}\right) \tag{7.17}
\end{equation*}
$$

\]

The coefficient $g_{(T)}$ measures the difference from the real cross section of the nuclide with respect to a $1 / v$ law while $s_{(T)}$ is the contribution to the reaction rate of the epithermal part of the spectrum from which the Maxwell distribution is


In this photograph from 1934 with Ernest Rutherford in the foreground, Carl Westcott is the young man walking by in the background. (Public Domain)
subtracted (Photo 7.4). The parameter $r$ normalizes the relative contributions from the epithermal and Maxwell distributions. It can be evaluated experimentally in a reactor using a fine sheet coated with cadmium. The activity is measured with and without cadmium Neutron fluence measurements (1970, p47). It can also be computed with a lattice code such as APOLLO using the method described at the end of this chapter. Westcott tabulated $s_{(T)}$ and $g_{(T)}$ for the absorption and fission cross sections of ${ }_{92}^{235} \mathrm{U},{ }_{94}^{239} \mathrm{Pu},{ }_{94}^{240} \mathrm{Pu}$ and ${ }_{94}^{241} \mathrm{Pu}$, which allowed the calculation of isotopic depletion in water reactors at a time when the calculation of neutron spectra was not so precise but very costly (no computers, approximate knowledge of cross

## A SURVEY OF VALUES OF THE $2200 \mathrm{~m} / \mathrm{s}$ CONSTANTS FOR FOUR FISSILE NUCLIDES

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## INTERNATIONAL ATOMIC ENERGY AGENCY VIENNA, 1965

Photo 7.4 The work of Westcott et al. on cross sections at $2200 \mathrm{~m} / \mathrm{s}$ (IAEA, 1965) (The Marguet collection)
sections with energy, etc.). The significant advantage of the Westcott model is that it provides the order of magnitude of one-group cross sections with sufficient precision to perform relevant engineering calculations for fuel depletion.

### 7.16.1 Calculation of Reaction Rate in a Pure Thermal Spectrum

Westcott defined the effective microscopic cross section $\widehat{\sigma}$ such that:

$$
\int_{0}^{\infty} n(v) \sigma(v) v d v=\widehat{\sigma} \quad v_{0} \int_{0}^{\infty} n(v) d v
$$

where:
$v_{0}$ is the reference speed at thermal energy, i.e. $2200 \mathrm{~m} / \mathrm{s}$, for which the cross section $\sigma_{0}$ is given; the latter can be obtained in any nuclear cross section data bank;
$n(v)$ is the distribution of the neutron density per unit speed. The choice of distribution $n(v)$ will be discussed later. The normalization of $n(v)$ is given by: $\int_{0}^{\infty} n(v) d v=n$.
By definition, the reaction rate is: $R=\int_{0}^{\infty} \Phi(v) \Sigma(v) d v$ with $\Phi(v)=n(v) v$ where:

$$
\begin{aligned}
R & =\int_{0}^{\infty} n(v) v N \sigma(v) d v=N \int_{0}^{\infty} n(v) \sigma(v) v d v \\
& =N \widehat{\sigma} v_{0} \underbrace{\int_{0}^{\infty} n(v) d v}_{n}=N \widehat{\sigma} v_{0} n
\end{aligned}
$$

with $N$ being the concentration of the nuclide for which the reaction rate is computed. The effective macroscopic cross section is used, $\widehat{\Sigma}=N \widehat{\sigma}$, by analogy to $\Sigma=N \sigma$.

$$
R=\widehat{\Sigma} v_{0} n
$$

where $n$ is the total number of neutrons per unit volume. These notations are those proposed by C.H. Westcott, W.H. Walker and T.K. Alexander in 1959 to standardize presentations on the subject matter. We saw earlier in this chapter that the flux spectrum may be written as:

$$
\Phi(E)=\Phi_{t h}[\underbrace{\frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}}_{m(E)}+\underbrace{\frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}(k T)}{\left(\xi \Sigma_{s}-\Sigma_{a}(k T)\right)} \frac{\Delta\left(\xi^{E} / k T\right.}{E}}_{\text {Epithermal part }}]
$$

It should be noted that $\int_{0}^{\infty} m(E) d E=1$. Assuming a pure thermal spectrum, this turns out to be equivalent to conserving the Maxwell distribution of the flux only (i.e. $\left.\Delta \quad\left({ }^{E / k T}\right)=0\right)$ :

$$
\Phi(E)=\Phi_{t h} m(E)
$$

The flux spectrum $\Phi(E)$ can also be defined using the neutron density with:

$$
\left\{\begin{array}{c}
v(E)=\sqrt{\frac{2 E}{m}} \\
n(E)=\frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} \frac{e^{-\frac{E}{k T}}}{k T}\left(\frac{1}{2} m v^{2}=E\right)
\end{array}\right.
$$

Since $\quad \Phi_{t h}=\sqrt{\frac{8 k T}{\pi m}} n_{t h}=\bar{v} n_{t h}=\frac{2}{\sqrt{\pi}} \sqrt{\frac{T}{T_{0}}} v_{0} n_{t h}$, the following may be written:

$$
n_{t h} n(E) v(E)=n_{t h} \frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} \sqrt{\frac{2 E}{m}} \frac{e^{-\frac{E}{k t}}}{k T}=\frac{\Phi_{t h}}{\sqrt{\frac{8 k T}{\pi m}}} \frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} \sqrt{\frac{2 E}{m}} \frac{e^{-\frac{E}{k T}}}{k T}
$$

where: $n_{t h} n(E) v(E)=\Phi_{t h} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}$
The pure thermal flux can be written indifferently under the form of neutron energy:

$$
\Phi(E)=\Phi_{t h} m(E) \quad \Phi_{t h}=\bar{v} n_{t h} \quad m(E)=\frac{E}{(k T)^{2}} e^{-\frac{E}{k T}} \quad \int_{0}^{\infty} m(E) d E=1
$$

or speed:
$\Phi(E)=n_{t h} n(E) v(E) \quad n(E)=\frac{2}{\sqrt{\pi}} \sqrt{\frac{E}{k T}} \frac{1}{k T} e^{-\frac{E}{k T}} \quad \int_{0}^{\infty} n(E) d E=1 \quad v(E)=\sqrt{\frac{2 E}{m}}$

### 7.16.2 Definition of the Westcott Coefficient $\mathbf{g}_{(\mathrm{T})}$

The reaction rate is written as:

$$
R_{t h}=\int_{0}^{\infty} \Phi(E) \Sigma(E) d E=\int_{0}^{\infty} n_{t h} n(E) v(E) \Sigma(E) d E
$$

The first Westcott coefficient $g_{(T)}$ is such that:

$$
\widehat{\Sigma}=\Sigma_{0} g_{(T)} \quad \text { and } \quad R_{t h}=\widehat{\Sigma} v_{0} n_{t h}
$$

The notation $g_{(T)}$ indicates that this coefficient depends on the moderator temperature, but not on the nature of the moderator itself (i.e. for uranium, the same coefficient $g_{(T)}$ is obtained for a reactor moderated by light water, heavy water or carbon). Hence the simplicity of this model. The definition of $\widehat{\Sigma}$ is $R_{t h} \equiv \widehat{\Sigma} v_{0} n$, but in the present case, $n=n_{t h}$ for a pure thermal spectrum. The thermal reaction rate is then given by:

$$
R_{t h}=n_{t h} N \int_{0}^{\infty} n(E) v(E) \sigma(E) d E=\Sigma_{0} g_{(T)} v_{0} n_{t h}
$$

with $\Sigma_{0}=N \sigma_{0}, v(E)=\sqrt{\frac{2 E}{m}}, \quad v_{0}=\sqrt{\frac{2 E_{0}}{m}}$.
Thus giving the exact analytical formula of the coefficient $g_{(T)}$ :

$$
g_{(T)}=\frac{\int_{0}^{\infty} n(E) \sigma(E) \sqrt{E} d E}{\sigma_{0} \sqrt{E_{0}}}
$$

The previous expression allows the calculation of $g_{(T)}$ when the fine description of the cross section $\sigma(E)$ with energy (point wise) is known. At low energy ( $<0.1 \mathrm{eV}$ ), thanks to precise measurements of the fission cross sections of ${ }_{92}^{233} \mathrm{U},{ }_{92}^{235} \mathrm{U},{ }_{94}^{239} \mathrm{Pu}$ and ${ }_{94}^{241} \mathrm{Pu}$ carried out in the GELINA accelerator (GEel LINear Accelerator) at GEEL by C. Wagemans et al., $\left.g_{(T 0}=20.44{ }^{\circ} \mathrm{C}\right){ }^{19}$ was recalculated (Table 7.4) for the main fissile isotopes of uranium and plutonium. It

Table 7.4 Comparison of $\left.g_{(20.44}{ }^{\circ} \mathrm{C}\right)$ for the main fissile nuclides

| Reference $\left.\mathrm{g}_{(20.44}{ }^{\circ} \mathrm{C}\right)$ | ${ }_{92}^{233} \mathrm{U}$ | ${ }_{92}^{235} \mathrm{U}$ | ${ }_{94}^{239} \mathrm{Pu}$ | ${ }_{94}^{241} \mathrm{Pu}$ |
| :--- | :--- | :--- | :--- | :--- |
| ENDF/B5 | 0.9966 | 0.9775 | 1.0582 | 1.0452 |
| ENDF/B6 | 0.9955 | 0.9771 | 1.0563 | 1.0450 |
| Wagemans et al. (1990) | 0.9940 | 0.9760 | 1.0550 | 1.036 |

[^132]

Fig. 7.9 Value of the Westcott factor in terms of temperature, obtained by numerical integration for ${ }_{92}^{233} U,{ }_{92}^{235} U, \quad{ }_{94}^{239} \mathrm{Pu}$ et ${ }_{94}^{241} \mathrm{Pu}$, from C. Wagemans et al.
should be pointed out that the value of $g_{(T)}$ is completely determined by the shape of the cross section $\sigma(E)$ under 1 eV and that the part below 20 meV accounts for $30 \%$.

Extrapolation by a quadratic polynomial below 2 meV has further refined the results of $g_{(T)}$ in a part for which no measurement was previously available (the contribution of the shape of the cross section below 2 meV being 1.5\%) (Fig. 7.9).

Westcott proposed the following values for $g_{(T)}$ and $s_{(T)}$, which will be computed later, but which was introduced in Eq. (7.16) (Table 7.5):

The particular case of an isotope with a cross section having a $1 / v$ shape (e.g. boron) can be obtained analytically:

$$
\Sigma_{a}(E)=\Sigma_{a}\left(E_{0}\right) \frac{v_{0}}{v}=\Sigma_{a}\left(E_{0}\right) \frac{\sqrt{k T_{0}}}{\sqrt{E}}, \quad E_{0}=0.0253 \mathrm{eV}=k T_{0}=\frac{1}{2} m v_{0}^{2}
$$

The Maxwell-distributed flux spectrum, of level $\Phi_{t h}$, is given by:

$$
\Phi(E)=\Phi_{t h} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}
$$

The reaction rate is then computed as:

$$
\begin{equation*}
\text { Thermal reaction rate }: R_{\text {thermal }}=\Sigma_{a}\left(v_{0}\right) \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \Phi_{t h} \tag{7.18}
\end{equation*}
$$

Table 7.5 $g_{(T)}$ and $s_{(T)}$ for the absorption and fission cross sections for the main fissile isotopes (from Reactor Physics constants, ANL-5800)

| T ( ${ }^{\circ} \mathrm{C}$ ) | ${ }_{92}^{235} U$ |  |  |  | ${ }_{94}^{240} \mathrm{Pu}$ |  | ${ }_{94}^{239} \mathrm{Pu}$ |  |  |  | ${ }_{94}^{241} \mathrm{Pu}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Absorption |  | Fission |  | Absorption |  | Absorption |  | Fission |  | Fission |  |
|  | $g_{(T)}$ | $s_{(T)}$ | $g_{(T)}$ | $s_{(T)}$ | $g_{(T)}$ | $s_{(T)}$ | $g_{(T)}$ | $s_{(T)}$ | $g_{(T)}$ | $s_{(T)}$ | $g_{(T)}$ | $s_{(T)}$ |
| 20 | 0.9780 | 0.0602 | 0.9759 | -0.0358 | 1.0270 | 33.63 | 1.0723 | 2.290 | 1.0487 | 1.794 | 1.0437 | 1.0518 |
| 100 | 0.9610 | 0.1009 | 0.9581 | -0.0044 | 1.0518 | 37.88 | 1.1611 | 2.336 | 1.115 | 1.836 | 1.0945 | 0.7845 |
| 200 | 0.9457 | 0.1390 | 0.9411 | 0.0253 | 1.0823 | 42.58 | 1.3388 | 2.105 | 1.2528 | 1.653 | 1.1832 | 0.6161 |
| 300 | 0.9357 | 0.1626 | 0.9291 | 0.0431 | 1.1160 | 46.78 | 1.5895 | 1.519 | 1.4507 | 1.182 | 1.2920 | 0.3464 |
| 450 | 0.9273 | 0.1825 | 0.9177 | 0.0555 | 1.1744 | 52.40 | 2.0505 | 0.259 | 1.8182 | 0.166 | 1.4652 | -0.0727 |
| 600 | 0.9229 | 0.2024 | 0.9108 | 0.0669 | 1.2521 | 57.36 | 2.5321 | -0.900 | 2.2037 | -0.770 | 1.6207 | $-0.3612$ |
| 800 | 0.9182 | 0.2416 | 0.9036 | 0.0934 | 1.4478 | 63.07 | 3.1006 | -1.928 | 2.6595 | -1.598 | 1.7758 | -0.5500 |
| 1000 | 0.9118 | 0.2910 | 0.8956 | 0.1304 | 1.9026 | 67.55 | 3.5353 | -2.532 | 3.0079 | -2.084 | 1.8693 | $-0.6040$ |
| 1300 | 0.8987 | 0.3717 | 0.8813 | 0.1935 | 3.5567 | 70.61 | 3.9419 | -2.998 | 3.3326 | -2.455 | 1.1986 | -0.5555 |

Using $\Phi_{t h}=\sqrt{\frac{8 k T}{\pi m}} n_{t h}$ and $v_{o}=\sqrt{\frac{2 k T_{o}}{m}}$ the following is deduced:

$$
R_{\text {thermal }}=\Sigma_{a}\left(v_{0}\right) v_{0} n_{t h}
$$

Defining the effective cross section $\widehat{\Sigma}_{a}$ such that $R=\widehat{\Sigma}_{a} \Phi_{t h}$, the following equation is obtained:

$$
\begin{equation*}
\text { Westcott effective cross section: } \widehat{\Sigma}_{a}=\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \Sigma_{a}\left(v_{0}\right) \tag{7.19}
\end{equation*}
$$

For example, the macroscopic cross section of graphite in the experimental Marius cold pile at the Marcoule (France) site was computed in 1959 as follows ${ }^{20}$ :

$$
\Sigma_{(n, \gamma)}^{\text {graphite }}=N_{\text {graphite }} \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}}\left[\sigma_{(n, \gamma)}^{\text {graphite }}+\frac{N_{\text {Nitrogen }}}{N_{\text {graphite }}} \frac{V_{\text {Nitrogen }}}{V_{\text {graphite }}} \sigma_{(n, \gamma)}^{\text {Nitrogen }}\right]
$$

with:
$N_{\text {graphite }}=\mathcal{N} \frac{\rho_{\text {graphite }}}{12.01}$
$N_{\text {Nitrogen }}=\mathcal{N} \frac{1}{11.20} \frac{p}{p_{0}} \frac{273.16}{T}$
$\rho_{\text {graphite }}=1.7 \mathrm{~g} / \mathrm{cm}^{3}$
$p_{0}=760 \mathrm{~mm} \mathrm{Hg}$
$T=19^{\circ} \mathrm{C}=291 \mathrm{~K}$
$V_{\text {Nitrogen }}$
the number of atoms in a mole of graphite
number of nitrogen atoms at pressure $p$ and temperature $T$
density of porous graphite (of reference density $\rho_{\text {graphite }}^{\text {ref }}=2.5 \mathrm{~g} / \mathrm{cm}^{3}$ )
reference pressure
room temperature of graphite
volume of nitrogen corresponding to the porosities of graphite of volume $V_{\text {graphite }}$

This calculation takes into account the capture of nitrogen in air ( $79 \%$ of air is composed of nitrogen) which fills up the porosities of graphite ( $\alpha=0.875$ ). The macroscopic cross section of nitrogen is far greater than that of graphite, and thus modifies the apparent cross section of graphite by taking into account the number of moles of air present:

$$
\frac{V_{\text {Nitrogen }}}{V_{\text {graphite }}}=\alpha \frac{\rho_{\text {graphite }}^{\text {ref }}-\rho_{\text {graphite }}}{\rho_{\text {graphite }}^{\text {ref }}} 79 \%
$$

[^133]Using a microscopic cross section of graphite at $2200 \mathrm{~m} / \mathrm{s}$ of $\sigma_{(n, \gamma)}^{\text {graphite }}=3.93$ mbarn and with the corresponding value for nitrogen under the same conditions being $\sigma_{(n, \gamma)}^{\text {nitrogen }}=1.88$ barn, the thermal cross section at room temperature ( $p=760 \mathrm{~mm} \mathrm{Hg}$ ) is:
$\sum_{(n, \gamma)}^{\text {graphite }}=3.12 \times 10^{-4} \mathrm{~cm}^{-1}$ i.e. normalized to an atom, $\sigma_{(n, \gamma)}^{\text {graphite }}=4.13 \mathrm{mbarn}$
This calculation uses an overrated value of the Avogadro number $\mathcal{N}=6.024$ $\times 10^{23} \mathrm{~mol}^{-1}$ that was prevalent at that time. The slowing-down cross section is evaluated using the formula:

$$
\Sigma_{r}^{\text {graphite }}=\frac{\overline{\xi \Sigma_{s}}}{u_{t h}-u_{0}}=\frac{\overline{\xi \Sigma_{s}}}{\ln \frac{E_{0}}{E_{t h}}} \approx \frac{0.0634 \mathrm{~cm}^{-1}}{18.2}=0.003483 \mathrm{~cm}^{-1}
$$

The thermal scattering area is computed as follows:

$$
L_{t h}^{2}=\frac{1}{3 \sum_{(n, \gamma)}^{\text {graphite }} \sum_{t}^{\text {graphite }}}=\frac{1}{33.1210^{-4} 0.416} \approx 2568 \mathrm{~cm}^{2}
$$

The slowing-down area has been determined from a slowing-down area of $376 \mathrm{~cm}^{2}$ for graphite of density $1.6 \mathrm{~g} / \mathrm{cm}^{3}$, i.e.:

$$
L_{r}^{2}=376\left(\frac{1,6}{\rho_{\text {graphite }}}\right)^{2} \approx 333 \mathrm{~cm}^{2}
$$

Since the migration area is the sum of the previous two areas, we find:

$$
M^{2}=L_{t h}^{2}+L_{r}^{2} \approx 2900 \mathrm{~cm}^{2}
$$

The thermal diffusion coefficient is given by:

$$
D_{2}=\Sigma_{(n, \gamma)}^{\text {graphite }} L_{t h}^{2} \approx 0.802 \mathrm{~cm}
$$

while the fast component is:

$$
D_{1}=\Sigma_{r}^{\text {graphite }} L_{r}^{2} \approx 1.16 \mathrm{~cm}
$$

### 7.17 Calculation of the Reaction Rate in a True Thermal Spectrum

In this case, the flux is not a pure Maxwell distribution but has an epithermal component:

True thermal spectrum : $\Phi(E)=\Phi_{t h} m(E)+\Phi_{\text {epithermal }}(E) \Delta\left(\frac{E}{k T}\right)$
where: $\Delta\left({ }^{E} / k T\right)$ is the junction function between a Maxwell-distributed flux and the epithermal flux $\Phi_{\text {epithermal }}(E)$

Let us consider a Maxwell-distributed flux completed by a junction function to the epithermal flux with a $1 / E$ shape.

$$
\Phi(E)=\Phi_{t h} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}+\Phi_{t h} \frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}(k T)}{\xi \Sigma_{S}-\Sigma_{a}(k T)} \frac{\Delta\left(\frac{E}{k T}\right)}{E}
$$

where:
$\lambda$ is a dimensionless coefficient of the junction function $\approx \frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}(k T)}{\xi \Sigma_{S}-\Sigma_{a}(k T)}$
$\Phi_{\text {epi } i}$ is the epithermal flux level in [neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$ ], i.e. $\Phi_{t h} \frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}(k T)}{\xi \Sigma_{S}-\Sigma_{a}(k T)}$. Care
must be taken to avoid confusion between $\Phi_{\text {epi }}$ in [neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$ ] and the
spectrum $\Phi_{\text {epithermal }}(E)=\Phi_{\text {epi }} / E$ in [neutrons $/ \mathrm{cm}^{2} / \mathrm{s} / \mathrm{eV}$ ]
$\Phi_{t h}$ is the thermal flux level: $\Phi_{t h}=n_{t h} \sqrt{\frac{8 k T}{\pi m_{\text {neurron }}}}$
The absorption rate associated with the corresponding cross section is:

$$
R=\int_{0}^{\infty} \quad \Sigma_{a}(E) \Phi(E) d E
$$

The neutron density per unit speed is given by:

$$
\begin{equation*}
\text { Neutron density : } n(v)=n(1-f) \rho_{m}(v)+n f \rho_{e}(v) \tag{7.21}
\end{equation*}
$$

where: $\rho_{m}(v)$ is the Maxwell distribution of neutron density;

$$
\rho_{m}(v)=\frac{4}{\sqrt{\pi}} \frac{v^{2}}{v_{T}^{3}} e^{-\left(\frac{v}{v_{T}}\right)^{2}}
$$

already encountered in the Boltzmann theory of gases under the term "distribution of speeds $p(v)$ ". By construction $\int_{0}^{\infty} \rho_{m}(v) d v=1$;
$\rho_{e}(v)$ is the distribution of the epithermal neutron density.
Fraction $f$ is the fraction of epithermal neutrons by (Bekurts and Wirtz 1964, p280): $f \equiv \frac{n_{e p i}}{n}$ thus $1-f \equiv \frac{n_{t h}}{n}$

The junction function $\Delta(E / k T)$ is simplified as a unit step function that is worth zero below $E / k T=\mu_{[-]}$, and equal to unity above. In reactor calculations at two energy groups, the thermal cut-off between the fast and thermal groups is chosen close to this value $\mu$, which gives an additional meaning to this value (Fig. 7.10). The value of $\mu$ is around 5 for light water reactors. Initially, a value of 4 was chosen to simplify the following integral calculation:

Fig. 7.10 Step junction function between the thermal and epithermal zones


$$
\int_{0}^{\infty} \Delta\left(\frac{E}{k T}\right)\left(\frac{k T}{E}\right)^{\frac{3}{2}} \frac{d E}{k T} \approx \int_{4}^{\infty} \Delta(x) \frac{1}{x^{\frac{3}{2}}} d x=1
$$

Under this hypothesis of the form $\Delta\left(\frac{E}{k T}\right)$, the epithermal density is computed as:

$$
\rho_{e}(v)=\frac{v_{T}}{v^{2}} \sqrt{\mu} \Delta\left(\frac{E}{k T}\right)
$$

meaning that the epithermal flux is of the shape $1 / E$ :

$$
\int_{0}^{\infty} \rho_{e}(v) d v=\int_{\mu}^{\infty} \frac{v_{T}}{v^{2}} \sqrt{\mu} d v \quad \text { and } \int_{0}^{\infty} \rho_{e}(v) d v=1
$$

Indeed: $\int_{0}^{\infty} \rho_{e}(v) d v=\int_{v_{(\mu)}}^{\infty} \frac{v_{T} \sqrt{\mu}}{v^{2}} d v=v_{T} \sqrt{\mu}\left[-\frac{1}{v}\right]_{v_{(\mu)}}^{\infty}=\frac{v_{T} \sqrt{\mu}}{v_{(\mu)}}$
$v_{(\mu)}$ is defined by $\frac{1}{2} m v_{(\mu)}^{2}=\mu k T$, thus: $v_{(\mu)}=\sqrt{2 \mu k T / m}$
hence, the epithermal normalization is equal to: $\int_{0}^{\infty} \rho_{e}(v) d v=\frac{v_{T}}{\sqrt{2 \mu k T / m}}$.
Since: $v_{T}=\sqrt{2 k T / m}$, the normalization verifies $\int_{0}^{\infty} \rho_{e}(v) d v=1$. Therefore, the following normalization equation is:

$$
\int_{0}^{\infty} n(v) d v=\int_{0}^{\infty}\left[n(1-f) \rho_{m}(v)+n f \rho_{e}(v)\right] d v=n
$$

Since, by definition $n(v)=n_{t h}(v)+n_{\text {epi }}(v)$ with $n_{t h}(v)=n_{t h} \rho_{m}(v)$ and $n_{\text {epi }}(v)=$ $n_{\text {epi }} \rho_{e}(v)$, it can be induced that $n_{t h}=n(1-f)$ and that $n_{\text {epi }}=n f$, thus, the coherence of the notation system.

### 7.17.1 Westcott Formalism: Introduction of the Coefficients r and s

The goal is to compute the absorption rate:

$$
R=\int_{0}^{\infty} \Sigma_{a}(E) \Phi(E) d E
$$

By substituting $\Phi(E)$ by its expression developed as $\Phi_{t h} m(E)+\Phi_{\text {epi }} \Delta\left(\frac{E}{k T}\right) / E$, we obtain:

$$
R=\underbrace{\int_{0}^{\infty} \Sigma_{a}(E) \Phi_{t h} m(E) d E}_{\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \Sigma_{0}\left(T_{0}\right) g_{(T)} \Phi_{t h}}+\int_{0}^{\infty} \Sigma_{a}(E) \Phi_{\text {epi }} \frac{\Delta\left(\frac{E}{k T}\right)}{E} d E
$$

Reaction rate $R$ is written as $\widehat{\Sigma}_{a} v_{0} n$ where $n=n_{t h}+n_{e p i}$ to introduce the effective cross section formulation after some algebraic calculations:

$$
n_{t h}=\frac{\Phi_{t h}}{\bar{v}}=\frac{\sqrt{\pi}}{2} \frac{\Phi_{t h}}{v_{T}}=\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \frac{\Phi_{t h}}{v_{0}}
$$

The goal is to express $n_{e p i}$ as a function of $\Phi_{\text {epi: }} \Phi_{e p i}(v)=\underbrace{n_{e p i} \rho_{e}(v)}_{n_{e p i}(v)} \cdot v$
where : $\int_{0}^{\infty} n_{e p i}(v) d v=\int_{0}^{\infty} n_{e p i} \rho_{e}(v) d v=n_{e p i}=\int_{0}^{\infty} \frac{\Phi_{\text {epi }}(E)}{v} d E=\int_{0}^{\infty} \frac{\Phi_{\text {epi }} \Delta\left(\frac{E}{k T}\right)}{v E} d E$
Since: $\int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E=\int_{\mu k T}^{\infty} \frac{1}{v E} d E=\sqrt{\frac{m}{2}}\left[-\frac{2}{\sqrt{E}}\right]_{\mu k T}^{\infty}=\sqrt{\frac{m}{2}} \frac{2}{\sqrt{\mu k T}}=\frac{2}{\sqrt{\mu}} \frac{1}{v_{T}}$
This calculation allows the evaluation of the number of epithermal neutrons:

$$
n_{e p i}=\Phi_{e p i} \int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E=\frac{2}{\sqrt{\mu}} \frac{\Phi_{e p i}}{v_{T}}
$$

Thus: $\widehat{\Sigma}_{a}=\frac{R}{v_{o} n}=\frac{\sqrt{\pi}}{2} \frac{\sqrt{\frac{T_{o}}{T}} \Sigma_{a\left(T_{o}\right)} g_{(T)} \Phi_{t h}}{v_{o} n}+\frac{\Phi_{e p i}}{v_{o} n} \int_{0}^{\infty} \Sigma_{a(T)} \frac{\Delta\left(\frac{E}{k T}\right)}{E} d E$
Since $\Phi_{t h}=\bar{v} n_{t h}$ and $\Phi_{e p i}=\frac{\sqrt{\mu} v_{T} n_{e p i}}{2}$, and by introducing the fraction $f$, the following is obtained:

$$
\widehat{\Sigma}_{a}=(1-f) g_{(T)} \Sigma_{a\left(T_{o}\right)} \underbrace{\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}} \frac{\bar{v}}{v_{o}}}_{1}+f \frac{\sqrt{\mu}}{2} \frac{v_{T}}{v_{o}} \int_{0}^{\infty} \Sigma_{a(T)} \frac{\Delta\left(\frac{E}{k T}\right)}{E} d E
$$

In the next equation, the following equations are used: $\bar{v}_{T}=\frac{2}{\sqrt{\pi}} v_{T}$ and $v_{T}$ $=\sqrt{\frac{T}{T_{o}}} v_{o}$ :

$$
\widehat{\Sigma}_{a}=(1-f) g_{(T)} \Sigma_{a\left(T_{o}\right)}+f \frac{\sqrt{\mu}}{2} \frac{v_{T}}{v_{o}} \int_{0}^{\infty} \Sigma_{a(T)} \frac{\Delta\left(\frac{E}{k T}\right)}{E} d E
$$

Yet by construction, $\int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E=\frac{2}{\sqrt{\mu}} \frac{1}{v_{T}}$ from the definition of $\mu$, hence:

$$
v_{o} \Sigma_{a\left(T_{o}\right)} \frac{\sqrt{\mu}}{2 v_{o}} \underbrace{v_{O} \sqrt{\frac{T}{T_{o}}}}_{v_{T}} \int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E=\Sigma_{a\left(T_{o}\right)}
$$

thus, by multiplying by $f g_{(T)}$ on both sides of the equation:

$$
f g_{(T)} \Sigma_{a\left(T_{o}\right)}=f g_{(T)} \frac{\sqrt{\mu}}{2} \frac{v_{T}}{v_{o}} \int_{0}^{\infty} \frac{v_{o} \Sigma_{a\left(T_{o}\right)} \Delta\left(\frac{E}{k T}\right)}{v E} d E
$$

which is substituted in the expression of $\widehat{\Sigma}_{a}$ :

$$
\widehat{\Sigma}_{a}=g_{(T)} \Sigma_{a\left(T_{o}\right)}+f \frac{\sqrt{\mu} v_{T}}{2 v_{o}} \int_{0}^{\infty}\left[\Sigma_{a(T)}-g_{(T)} \frac{\Sigma_{a(o)} v_{o}}{v}\right] \frac{\Delta\left(\frac{E}{k T}\right)}{E} d E
$$

Let $N_{a}$ be the number of absorbing nuclides (Bekurts and Wirtz 1964, p280):

$$
\widehat{\Sigma}_{a}=g_{(T)} \Sigma_{a(o)}+f \frac{\sqrt{\mu}}{2} \frac{v_{T}}{v_{o}} N_{a} I^{\prime}
$$

defining the excess resonance integral as:

$$
\begin{equation*}
\text { Excess resonance integral }: I^{\prime} \equiv \int_{0}^{\infty}\left[\sigma_{a}-g_{(T)} \frac{\sigma_{a(o)} v_{o}}{v}\right] \frac{\Delta\left(\frac{E}{k T}\right)}{E} d E \tag{7.22}
\end{equation*}
$$

The excess resonance integral counts as positive the areas above the line $1 / v$ (in logarithmic scale) and as negative the areas below, hence its name. Defining the second Westcott coefficient and the spectrum index by:

$$
s_{(T)[-]} \equiv \frac{1}{\sigma_{a\left(v_{o}\right)}} \frac{2}{\sqrt{\pi}} \sqrt{\frac{T}{T_{o}}} I^{\prime} \quad \text { and } \quad r_{[-]} \equiv f \frac{\sqrt{\pi \mu}}{4}
$$

Since $f \equiv \frac{n_{e p i}}{n}=\frac{n_{e p i}}{n_{e p i}+n_{t h}}$, the Westcott spectrum index is given by:

$$
\begin{equation*}
\text { Westcott spectrum index : } r=\frac{\frac{\sqrt{\pi \mu}}{4}}{1+\frac{\sqrt{\pi \mu}}{4}} \frac{\Phi_{l h}}{\Phi_{e} p i} \tag{7.23}
\end{equation*}
$$

In the case of water reactors, the epithermal flux is small compared to the thermal flux, hence the simplification of the spectrum index as:

$$
\Phi_{e p i} \ll \Phi_{t h} \quad \Rightarrow \quad r \approx \frac{\Phi_{e p i}}{\Phi_{t h}}=\lambda=\frac{\sqrt{\pi}}{2} \frac{\Sigma_{a(T)}}{\xi \Sigma_{S}-\Sigma_{a(T)}}
$$

Since homogeneous absorption is insignificant compared to the slowing-down power of well-thermalized media:

$$
\Sigma_{a} \ll \xi \Sigma_{s} \quad \Rightarrow \quad r \approx \frac{\sqrt{\pi}}{2} \frac{\Sigma_{a(k T)}}{\xi \Sigma_{S}} \approx \lambda
$$

There is approximate equality between the epithermal ratio $r$ and the junction fraction $\lambda$. By mathematical manipulation of equations, the spectrum index is introduced in the formula of the effective cross section:

$$
\begin{gathered}
\widehat{\Sigma}_{a}=g_{(T)} N_{a} \sigma_{a(o)}+f \frac{\sqrt{\mu}}{2} \frac{v_{T}}{v} N_{a} I^{\prime} \\
\widehat{\Sigma}_{a}=N_{a} \sigma_{a(o)}[g_{(T)}+\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}} \sigma_{a\left(T_{o}\right)} \underbrace{\frac{1}{\sigma_{a\left(T_{o}\right)}} \frac{2}{\sqrt{\pi}} \sqrt{\frac{T}{T_{o}}} I^{\prime}}_{s_{(T)}} \begin{array}{l}
\underbrace{\frac{\frac{\sqrt{\pi \mu}}{4}}{1+\frac{\sqrt{\pi \mu}}{4} \frac{\Phi_{t h}}{\Phi_{\grave{e} p i}}}}_{r}]
\end{array}]
\end{gathered}
$$

Or even: $\widehat{\Sigma}_{a}=g_{(T)} N_{a} \sigma_{a(o)}+\frac{2}{\sqrt{\pi}} r \frac{v_{T}}{v_{0}} I^{\prime}$
Since ${ }^{v T} / \nu_{0}=\sqrt{T / T_{0}}$, the calculation of the effective cross section is simplified to:

$$
\widehat{\Sigma}_{a}=g_{(T)} N_{a} \sigma_{a(o)}+N_{a} \sigma_{a(o)} r s_{(T)}
$$

Hence, the conventional Westcott formula:

Westcott formula: $\widehat{\Sigma}_{a}=N_{a} \sigma_{a(o)}\left[g_{(T)}+r s_{(T)}\right] \quad$ and $\quad R=\widehat{\Sigma}_{a} v_{o} n$
Since: $v_{o}=\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}} \bar{v}$ and $\Phi_{t h}=n_{t h} \bar{v}$, the following equation can also be written:

$$
R=N_{a} \sigma_{a(o)} \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}}\left[g_{(T)}+r s\right] \Phi_{t h} \frac{n}{n_{t h}}
$$

Since: $f=\frac{1}{1+\frac{n_{h}}{n_{e p i}}}$ and $\frac{n_{e p i}}{n_{t h}}=1+\frac{\frac{2}{\sqrt{\mu}} \frac{\Phi_{e p i}}{v_{T}}}{\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \frac{\varphi_{\rho_{h}}}{v_{0}}}=\frac{4}{\sqrt{\pi \mu}} \frac{\Phi_{e p i}}{\Phi_{t h}}$,

$$
\frac{n}{n_{t h}}=\frac{n_{e p i}+n_{t h}}{n_{t h}}=1+\frac{n_{e p i}}{n_{t h}}=1+\frac{4}{\sqrt{\pi \mu}} \frac{\Phi_{e p i}}{\Phi_{t h}}
$$

The absorption rate is expressed as:

$$
R=N_{a}\left[\sigma_{a(o)} \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}} g_{(T)}+r I^{\prime}\right] \Phi_{t h}\left(1+\frac{4}{\sqrt{\pi \mu}} \frac{\Phi_{\hat{e} p i}}{\Phi_{t h}}\right)
$$

In a $P W R$ with $3.7 \% \mathrm{U} 235$,

$$
\frac{\Phi_{e p i}}{\Phi_{t h}} \approx 0.3, \frac{n}{n_{t h}} \approx 1, R \approx N_{a} \sigma_{a(o)} \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}}\left[g_{(T)}+r s_{(T)}\right] \Phi_{t h}
$$

Since $s_{(T)}=\frac{1}{\sigma_{a\left(v_{o}\right)}} \frac{2}{\sqrt{\pi}} \sqrt{\frac{T}{T_{o}} I^{\prime}}$ :
Simplified Westcott formula for a thermal spectrum:

$$
\begin{equation*}
R \approx N_{a}\left[\sigma_{a(o)} \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{o}}{T}} g_{(T)}+r I^{\prime}\right] \Phi_{t h} \tag{7.25}
\end{equation*}
$$

with the approximation: $\frac{4}{\sqrt{\pi \mu}} \frac{\Phi_{e p i}}{\Phi_{t h}} \ll 1$ and $r=\frac{\frac{\sqrt{\pi \mu}}{4}}{1+\frac{\Phi^{\prime} \mu}{4}} \frac{\frac{\varphi}{t h}^{\Phi_{e p i}}}{\Phi_{e p i}} \frac{\Phi_{t h}}{\Phi_{t h}}$
The excess resonance integral $I^{\prime}$ must not be confused with the usual resonance integral $I$ :

$$
I^{\prime} \equiv I-g_{(T)} \int_{E_{c}}^{\infty}\left(\frac{\sigma_{a}\left(v_{0}\right) v_{o}}{v}\right) \frac{1}{E} d E \quad I \equiv \int_{0}^{\infty} \sigma_{a}(u) d u=\int_{0}^{\infty} \frac{\sigma_{a}(E) d E}{E}
$$

which is found in nuclear data libraries or compilations (books) of nuclear data, and which is usually given as between 0.5 eV and $100 \mathrm{keV}\left(I=\int_{0.5 \mathrm{eV}}^{100 \mathrm{keV}} \sigma_{a}(u) d u\right)$. Indeed, the excess resonance can be negative for nuclides for which the cross section is well below the line $\sigma_{a}\left(v_{0}\right) \quad v_{o} / v$ (on a logarithmic energy scale). For a cross section which is a pure $1 / v$ cross section, the excess resonance integral is zero. In a $P W R, \Delta \quad\left(E_{c} / k T\right)=0$ when $\mu=E_{c} / k T \leq 4$ or 5 . Using the Boltzmann constant $k=1.38065810^{-23} \mathrm{~J} \mathrm{~K}^{-1}$ and for a moderator temperature of $T_{\text {mod }}=306{ }^{\circ} \mathrm{C}=$ 579.15 K i.e. $k T \approx 0.05 \mathrm{eV}$, the epithermal component is zero below 0.2 eV . It should be noted that the Westcott formalism is valid not only for computing the capture cross section of fission products but also the fission cross section of heavy nuclides.

### 7.17.2 Extension of the Model to Other Nuclides: The Linear Logarithmic Model

The Westcott formalism proposes tabulated values for the coefficients $g_{(T)}$ and $s_{(T)}$ for $U_{235}^{\text {fission }}, U_{235}^{\text {absorption }}, P u_{239}^{\text {fission }}, P u_{239}^{\text {absorption }}, P u_{241}^{\text {fission }}$ and $P u_{241}^{\text {absorption }}$. However, few coefficients are available for fission products, particularly for those with resonances. A more general formalism was sought, such that it might be applied to all nuclides not verifying the $1 / v$ law. In general, the absorber cross sections do not verify this $1 / v$ law, even though the $\ln \left(\sigma / \sigma_{0}\right)$ law with respect to $\operatorname{In}\left(v / v_{0}\right)$ is a line at low energy (except for nuclides with resonances in the thermal zone). Assuming that the $\ln \left(\sigma / \sigma_{0}\right)$ law has a deviation from the $1 / v$ law with an angle $d \alpha$ (cf. Fig. 7.11), if $\sigma$ obeys a $1 / v$ law, then: $\sigma=\sigma_{0} v_{0} / v$, hence:

Fig. 7.11 Deviation from the $1 / v$ law


$$
\ln \left(\frac{\sigma}{\sigma_{0}}\right)=-\ln \left(\frac{v}{v_{0}}\right)
$$

Let $Y \equiv \ln \left(\frac{\sigma}{\sigma_{0}}\right)$ and $X \equiv \ln \left(\frac{v}{v_{0}}\right)$. Using the properties of the tangent of an angle:

$$
\tan \alpha=-1=-\frac{X}{Y} \quad \text { and } \quad \tan (\alpha+d \alpha)=\frac{Y}{X}
$$

Therefore: $\tan (\alpha+d \alpha)-\tan \alpha=\frac{Y+X}{X}$
By differentiating: $\frac{d(\tan \alpha)}{d \alpha}=1+\tan ^{2} \alpha=\frac{\tan (\alpha+d \alpha)-\tan \alpha}{d \alpha}$ if $d \alpha$ is small.
Moreover: $\tan \alpha=\tan \left(-45^{\circ}\right)=-1,\left(1+\tan ^{2} \alpha\right) d \alpha=\frac{Y+X}{X}$ thus: $2 X d \alpha=Y+X$ Furthermore: $Y=\ln \left(\sigma / \sigma_{0}\right)$ and $X=\ln \left(v / v_{0}\right)$, we obtain:

$$
\ln \left(\frac{\sigma}{\sigma_{0}}\right)=(2 d \alpha-1) \ln \frac{v}{v_{0}}
$$

thus, when $d \alpha$ is small (and in any case, much smaller than 0.5 radian):
Shape of the linear cross section with a logarithmic scale: $\sigma=\sigma_{0}\left(\frac{v_{0}}{v}\right)^{1-2 d \alpha}$

The reaction rate corresponding to such a cross section is computed as follows:

$$
R=\int_{0}^{\infty} \Sigma_{a}(v) \Phi_{t h} m(E) d E=\int_{0}^{\infty} \Sigma_{a}(0)\left(\frac{v_{0}}{v}\right)^{1-2 d \alpha} \Phi_{t h} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}} d E
$$

Since: $\frac{v_{0}}{v}=\sqrt{\frac{E_{0}}{E}}=\sqrt{\frac{k T_{0}}{E}}$, we obtain:

$$
\begin{aligned}
R & =\Sigma_{a}(0) \Phi_{t h} \int_{0}^{\infty}\left(\frac{k T_{0}}{E}\right)^{\frac{1-2 d \alpha}{2}} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}} d E \\
& =\Sigma_{a}(0) \Phi_{t h} \sqrt{\frac{T_{0}}{T}} \int_{0}^{\infty}\left(\frac{T}{T_{0}}\right)^{d \alpha}\left(\frac{E}{k T}\right)^{\frac{1}{2}+d \alpha} e^{-\frac{E}{k T}} \frac{d E}{k T}
\end{aligned}
$$

We wish to introduce $\sqrt{T_{0} / T}$ in front of the integral term, just as in the simple Westcott formalism in the thermal spectrum. By identifying the integral with the real factorial $\Gamma(x)=\int_{0}^{\infty} t^{x-1} e^{-t} d t$ term, with the variable substitution $x=E / k T$, the following equation is reached:

$$
R=\Sigma_{a}(0) \Phi_{t h} \sqrt{\frac{T_{0}}{T}}\left(\frac{T}{T_{0}}\right)^{d \alpha} \Gamma\left(\frac{3}{2}+d \alpha\right)
$$

Since $\Gamma(3 / 2)=\sqrt{\pi} / 2$, the Westcott reaction rate for a $1 / v$ cross section in thermal spectrum can be introduced:

$$
R=\Sigma_{a}(0) \frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T}} \Phi_{t h}\left(\frac{T}{T_{0}}\right)^{d \alpha} \frac{\Gamma\left(\frac{3}{2}+d \alpha\right)}{\Gamma\left(\frac{3}{2}\right)}
$$

Hence, an analytical formula for the Westcott coefficient $g_{(T)}$ is obtained under the assumption of a deviation $d \alpha$ characteristic of the nuclide being considered (Marguet, 2002):

$$
g_{W-M(T)}=\left(\frac{T}{T_{0}}\right)^{d \alpha} \frac{\Gamma\left(\frac{3}{2}+d \alpha\right)}{\Gamma\left(\frac{3}{2}\right)}
$$

This model may be extended to the general case when the curve for the cross section can be approximated by successive lines of variable gradients. It is the case for giant resonances such as that at 0.067 eV for ${ }^{135} \mathrm{Xe}$, which are characterized by a $1 / v$ gradient on the left of the resonance and $1 / v^{5}$ on the right. The calculation of the capture rate of this particular resonance is of the utmost importance in $P W R$. Since this resonance is also large, it is not subject to the Doppler effect, and the capture rate of ${ }^{135} \mathrm{Xe}$ may be computed analytically using the approach described previously.

The work of Cohen et al. further showed ${ }^{21}$ that the epithermal spectrum may be modeled empirically using the following form:

$$
\Phi_{\text {epithermal }}(E)=\frac{\Phi(1 \mathrm{eV})(1 \mathrm{eV})^{1+\beta}}{E^{1+\beta}}
$$

This model leads to the calculation of the resonance integral under the form given below, with $E_{\text {cut-off }} \approx 0.1$ to 0.2 eV being the thermal/epithermal cut-off:

$$
I(\beta)=\int_{E_{\text {cut-off }}}^{\infty} \frac{\sigma(E)(1 \mathrm{eV})^{1+\beta}}{E^{1+\beta}} d E
$$

The use of our form of the cross section, $\sigma=\sigma_{0}\left(E_{0} / E\right)^{\frac{1-2 d \alpha}{2}}$, leads to an analytical calculation of $I(\beta)$.

[^134]Fig. 7.12 Progressive junction at the epithermal zone


### 7.17.3 Progressive Junction at Epithermal Energy

Assuming that the junction function $\Delta\left({ }^{E} / k T\right)$ is more complex than a step function, for instance a linear junction function (Fig. 7.12). Thus:

$$
n_{e p i}=\int_{0}^{\infty} \frac{\Phi_{e p i} \Delta\left(\frac{E}{k T}\right)}{v E} d E
$$

Since : $\quad \int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E=\int_{\mu_{1} k T}^{\mu_{2} k T} \frac{\frac{E}{k T}-\mu_{1}}{\mu_{2}-\mu_{1}} \frac{v E}{v} d E+\int_{\mu_{2} k T}^{\infty} \frac{1}{v E} d E$
from which: $\int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E=\frac{2}{\sqrt{\mu_{1}}+\sqrt{\mu_{2}}} \frac{2}{v_{T}}=\frac{1}{K_{\mu}} \frac{2}{v_{T}}$
In the standard Westcott model with a step junction function, the following is obtained:

$$
\Phi_{e p i}=\frac{n_{e ́ p i}}{\int_{0}^{\infty} \frac{\Delta\left(\frac{E}{k T}\right)}{v E} d E}=\frac{\sqrt{\mu} v_{T}}{2} n_{e p i}
$$

i.e. a particular value of $K_{\mu}: K_{\mu}=\sqrt{\mu}$. The Westcott equations can be generalized by setting:

$$
r=f \frac{\sqrt{\pi} K_{\mu}}{4}=\frac{\frac{\sqrt{\pi}}{4} K_{\mu}}{1+\frac{\sqrt{\pi}}{4} K_{\mu} \frac{\Phi_{t h}}{\Phi_{e p i}}} \text { with } K_{\mu}=\frac{\sqrt{\mu_{1}}+\sqrt{\mu_{2}}}{2} \text { and } \mu_{1}=\mu_{2}
$$

for a step junction. Such an approach is limited by the fact that in practice, the junction function depends on the thermal absorption level: thus, the junction is different depending on the boron level in the moderator of a $P W R$.

### 7.17.4 Westcott Junction

In 1960, Westcott proposed ${ }^{22}$ an epithermal junction given under the following form:

Westcott neutron density: $n(v)$

$$
\begin{equation*}
=n \frac{4}{\sqrt{\pi}}\left(\left(1-\frac{4 r}{\sqrt{\pi}} \int_{0}^{\infty} \frac{v_{T}}{v^{2}} \Delta(v) d v\right) \frac{v^{2}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{3}}}+r \frac{v_{T}}{v^{2}} \Delta(v)\right) \tag{7.27}
\end{equation*}
$$

where $v_{T}=\sqrt{T / T_{0}} v_{0}$ is the most probable speed of the Maxwell spectrum, $\Delta(v)$ is the cut-off function encountered earlier and $r$ is the usual epithermal spectrum index. The condition $\int_{0}^{\infty} n(v) d v=n$ gives the normalization of the function $\Delta(v)$. In the above formula, we have the pure Maxwell part:

$$
m(v)=n \frac{4}{\sqrt{\pi}} \frac{v^{2}}{v_{T}^{3}} e^{-\frac{v^{2}}{v_{T}^{3}}}
$$

as well as the neutron density junction function that includes the cut-off function $\Delta(v)$. Introduction of the reduced speed $x_{[-]} \equiv v / v_{T} \quad$ (hence, $d x_{[-]}=d v / v_{T}$ ) leads to the following equation:

$$
\begin{aligned}
n(v) d v & =n \frac{4}{\sqrt{\pi}}\left(\left(1-\frac{4 r}{\sqrt{\pi}} \int_{0}^{\infty} \frac{1}{x^{2}} \Delta d x\right) \frac{x^{2}}{v_{T}} e^{-x^{2}}+r \frac{v_{T}}{v^{2}} \Delta\right) v_{T} d x \\
& =n \frac{4}{\sqrt{\pi}}\left(\left(1-\frac{4 r}{\sqrt{\pi}} \int_{0}^{\infty} \frac{1}{x^{2}} \Delta d x\right) x^{2} e^{-x^{2}}+r \frac{1}{x^{2}} \Delta\right) d x=n(x) d x
\end{aligned}
$$

thereby:
$n(x)=n \frac{4}{\sqrt{\pi}}\left(\left(1-\frac{4 r}{\sqrt{\pi}} \int_{0}^{\infty} \frac{1}{x^{2}} \Delta d x\right) x^{2} e^{-x^{2}}+r \frac{1}{x^{2}} \Delta\right)=n \frac{4}{\sqrt{\pi}}\left((1-r b) x^{2} e^{-x^{2}}+r \frac{1}{x^{2}} \Delta\right)$
with $b=\frac{4}{\sqrt{\pi}} \int_{0}^{\infty} \frac{1}{x^{2}} \Delta d x$
The junction function satisfies the following conditions:

$$
\lim _{x \rightarrow 0}\left(\frac{1}{x^{2}} \Delta(x)\right)=0 \quad \text { and } \quad \lim _{x \rightarrow \infty}\left(\frac{1}{x^{2}} \Delta(x)\right)=1
$$

The integral calculated over the complete spectrum results in:

[^135]\[

$$
\begin{aligned}
\int_{0}^{\infty} n(x) d x & =\int_{0}^{\infty} n \frac{4}{\sqrt{\pi}}\left((1-r b) x^{2} e^{-x^{2}}+r \frac{1}{x^{2}} \Delta\right) \\
& =n(1-r b) \frac{4}{\sqrt{\pi}} \underbrace{\int_{0}^{\infty} x^{2} e^{-x^{2}}}_{\frac{r\left(\frac{3}{2}\right)}{2}=\frac{\sqrt{\pi}}{4}}+n r \underbrace{\frac{4}{\sqrt{\pi}} \int_{0}^{\infty} \frac{1}{x^{2}} \Delta d x}_{b}=n
\end{aligned}
$$
\]

Westcott proposed several empirical cut-off functions that lead to different values of $s_{(T)}$ :

$$
\begin{cases}\Delta_{1}(v)=\frac{1}{1+\left(3.5 \frac{v_{T}^{2}}{v^{2}}\right)^{7}} & \text { hence } b_{1}=1.216414 \pm 0.000001 \\ \Delta_{2}(v)=\frac{1}{1+\left(4.95 \frac{v_{T}^{2}}{v^{2}}\right)^{7}} & \text { hence } b_{2}=1.022876 \pm 0.000001 \\ \Delta_{3}(v)=\frac{1}{1-\frac{0,26}{1+(2.131 . E)^{5}}} \frac{1}{1+\left(4.95 \frac{v_{T}^{2}}{v^{2}}\right)^{7}} & \text { hence } b_{3} \text { depends on } T \\ \Delta_{4}(v)=\frac{1}{1-\frac{0,26}{1+\left(\frac{E}{16.4 k T}\right)^{5}}} \frac{1}{1+\left(4.75 \frac{v_{T}^{2}}{v^{2}}\right)^{7}} \text { hence } b_{4}=1.176246 \pm 0.000001\end{cases}
$$

The value of $b$ enables calculation of the equivalent reduced cut-off energy $\mu$ for which the junction function is a step function. Since $b=4 / \sqrt{\pi \mu}$ in this latter case, we obtain $\mu_{1}=3.442, \mu_{2}=4.848$ and $\mu_{4}=3.681$. $\mu_{3}$ varies from 3.600 at $20^{\circ} \mathrm{C}$ up to 4.478 at $606^{\circ} \mathrm{C}$. The order of magnitude corresponding to 4 or 5 used in previous sections to simplify the integral calculations is thus explained. The empirical formulae for $\Delta(v)$ may be summarized as:

$$
\Delta(x)=\frac{1}{1+\left(\mu x^{-2}\right)^{m}} \quad \text { where } m \text { is approximately equal to } 7
$$

### 7.17.5 Determination of Cut-Off Function

Earlier, it was stated that in slowing-down theory without absorption, the flux is equal to:

$$
\Phi(E)_{[\mathrm{n} / \mathrm{cm} / \mathrm{s} / \mathrm{s} / \mathrm{eV}]}=n(E) v(E)=\frac{Q_{\left[\mathrm{n} / \mathrm{cm}^{3} / \mathrm{s}\right]}}{\xi \sum_{s\left[\mathrm{~cm}^{-1}\right]} E_{[\mathrm{ev}]}}
$$

Using $E=m v^{2} / 2=m v_{T}^{2} x^{2} / 2$ and the fact that $n(E) d E=n(x) d x$, the neutron density in terms of the reduced speed is:

$$
n(x)=\frac{Q}{v_{T} \xi \Sigma_{s}} \quad \frac{2}{x^{2}}
$$

When the reduced speed is sufficiently great, the neutron density is:

$$
n(x)=n \frac{4}{\sqrt{\pi}}\left((1-r b) x^{2} e^{-x^{2}}+r \frac{1}{x^{2}} \Delta\right)
$$

and tends towards $n(x)=n \frac{4}{\sqrt{\pi}}\left(r \frac{1}{x^{2}}\right) d x$.
Thus, the expression of $r$ obtained by identification is: $r=\frac{\sqrt{\pi}}{2} \frac{Q}{v_{T} \xi \Sigma_{s}}$ (Fig. 7.13).


Fig. 7.13 Junction functions from Westcott

In the steady state, it can be assumed that all neutrons emitted are absorbed during slowing-down and thermalization (supposing that leakage is disregarded, i.e. in infinite medium):

$$
Q_{\left[\mathrm{n} / \mathrm{cm}^{3} / \mathrm{s}\right]}=\Sigma_{a\left[\mathrm{~cm}^{-1}\right]}(n v)_{\left[\mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}\right]}=\widehat{\Sigma}_{a} n v_{0}
$$

Thereby:

$$
r=\frac{\sqrt{\pi}}{2} \frac{\widehat{\Sigma}_{a} n v_{0}}{n v_{T} \xi \Sigma_{s}}=\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0} \widehat{\Sigma}_{a}}{T \xi \Sigma_{s}}}
$$

This result was previously demonstrated for the junction coefficient of the epithermal function. Finally, the Westcott formalism is written in shorthand form:

$$
\left\{\begin{array}{l}
\widehat{\sigma}=\sigma_{0}\left(g_{(T)}+r s_{(T)}\right) \quad \text { with } r=\frac{\sqrt{\pi}}{2} \sqrt{\frac{T_{0}}{T} \frac{\Sigma_{a}}{\xi \Sigma_{s}}} \\
g_{(T)}=\sqrt{\frac{T_{0}}{T}} \frac{1}{\sigma_{0}} \int_{O}^{\infty} \sigma(x) \frac{4}{\sqrt{\pi}} x^{2} e^{-x^{2}} x d x \quad s_{(T)}=\frac{2}{\sqrt{\pi}} \sqrt{\frac{T}{T_{0}}} \frac{1}{\sigma_{0}} \int_{O}^{\infty} \sigma(x) \Delta(x) \frac{2}{x^{2}} x d x-b g_{(T)}
\end{array}\right.
$$

### 7.17.6 Limits of the Westcott Formalism

One of the main qualities of the Westcott formalism is its relative simplicity. The coefficients $g_{(T)}$ and $s_{(T)}$ depend solely on the temperature and the fissile nuclides, and not on the nature of the moderator. However, it has been pointed out that it requires that absorption be negligible compared to slowing-down such that the thermal spectrum has a Maxwell distribution. In practice, the deviation from this absorption-induced Maxwell distribution requires the use of a correction term on the temperature of the spectrum, a term that will depend on the moderator, thus rendering the model more limited. Historically, the Westcott model was largely employed to compute the absorption rate of nuclides for which the absorption cross section was not well known but the resonance integral and the value of $\sigma_{0}$ were. Today's updated and refined nuclear data banks have led to the use of multi-group calculations of reaction rate rather than recourse to the Westcott model. The one-group cross sections are thus obtained by:

$$
\left(\sum_{g} \Phi_{g}\right) \bar{\sigma}=\sum_{g} \sigma_{g} \Phi_{g}
$$

### 7.18 Application of the Westcott Formalism

The epithermal ratio $r$ and the Maxwell-distributed flux $\Phi_{t h}$ can be computed fairly easily with the Westcott formalism using results from the French transport code APOLLO1 for 99 energy groups condensed into four energy groups (macro-groups) that cover the thermal zone, epithermal domain and two fast groups. The bounds of the groups (in decreasing energy value) are:

| Group 1: $[10 \mathrm{MeV}, 0.907 \mathrm{MeV}]$ | Or in lethargy [0-2.4] | Groups [1,12] |
| :--- | :--- | :--- |
| Group 2: $[0.907 \mathrm{MeV}, 2.248 \mathrm{keV}]$ | Or in lethargy [2.4-8.4] | Groups [13,27] |
| Group 3: $[2.248 \mathrm{keV}, 0.625 \mathrm{eV}]$ | Or in lethargy [8.4-16.59] | Groups [27,75] |
| Group 4: $\left[0.625 \mathrm{eV}, 1.1 \times 10^{-4} \mathrm{eV}\right]$ | Or in lethargy [16.59-25.23] | Groups [76,99] |

Historically, this approach was used in depletion codes in France for calculating the cross sections of fission products for which only the cross sections at $2200 \mathrm{~m} / \mathrm{s}$ and the resonance integral were known. By the mid-1990s, with improved knowledge of the cross sections of fission products with energy, this method was superseded by a more precise condensation of multi-group cross sections from the flux spectrum of an assembly calculation. The cut-off of the 4th energy group $(0.625 \mathrm{eV})$ is the usual cut-off as that for two-group calculations for $P W R$, also called the cadmium cut-off (assuming that a cadmium sheet can absorb all neutrons under this threshold in a cadmium detector, which historically helped in characterizing the spectrum). The level of thermal flux is computed by expressing conservation of the fission rate of ${ }_{92}^{235} U$ in the last energy macro-group (the last thermal macro-group in the example given) and the reaction rate of the thermal Maxwelldistributed flux $\Phi_{t h}$ :

$$
\sigma_{\max w}\left({ }_{92}^{235} U\right) \cdot \Phi_{t h}=\sigma_{4}^{\text {fission }} \text { apollo }\left({ }_{92}^{235} U\right) \cdot \Phi_{4}
$$

The Maxwell cross section is defined by: $\sigma_{\max w}\left({ }_{92}^{235} U\right)=\sigma_{0}\left({ }_{92}^{235} U\right) \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}$. Consequently, an expression for the thermal flux is obtained:

$$
\Phi_{t h}=\frac{\sigma_{4}^{\text {fission }} \text { apollo }\left({ }_{92}^{235} U\right) \Phi_{4}}{\sigma_{0}\left({ }_{92}^{235} U\right) \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}}
$$

where $\Phi_{4}$ is the average APOLLO2 flux in macro-group 4 and $\sum_{g=1,4} \Phi_{g}$ is the sum of the APOLLO2 flux over the 4 energy macro-groups.

Numerical example: $\sigma_{0}\left({ }_{92}^{235} U\right)=583.2$ barns (fission, JEF2), $T_{0}=293.15 \mathrm{~K}$,
For water temperature: $T=T_{H_{2} 0}=578.45 \mathrm{~K}$. Thus:

Table 7.6 4-group data for a 3.7\% enriched fuel

| $\Phi_{g}\left[\right.$ neutron $\left./ \mathrm{cm}^{2} / \mathrm{s}\right]$ | 1 |  | 2 |  | 3 |  | 4 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Energy bounds |  | 0.90718 | 0.90718 | $2.10^{-03}$ | $2.10^{-03}$ | 0.625 | 0.625 | $1.1 \times 10^{-04}$ |
|  | MeV | MeV | MeV | MeV | MeV | eV | eV | eV |
| $0 \mathrm{MWd} /$ ton | $0.750710^{14}$ |  | $1.136810^{14}$ |  | $0.642910^{14}$ |  | $0.366110^{14}$ |  |
| 42,500 MWd/ton | $1.026310^{14}$ |  | $1.570010^{14}$ |  | $0.930910^{14}$ |  | $0.457110^{14}$ |  |
| Two-groups flux | $\Phi_{1}=\sum_{g=1,3} \Phi_{g}$ |  |  |  |  |  | $\Phi_{2}=\Phi_{4}$ |  |
| $0 \mathrm{MWd} /$ ton | $2.532810^{14}$ |  |  |  |  |  | $0.366210^{14}$ |  |
| 42,500 MWd/ton | $3.508110^{14}$ |  |  |  |  |  | $0.457110^{14}$ |  |
| One-group flux | $\sum_{g=1,4} \Phi_{g}$ |  |  |  |  |  |  |  |
| $0 \mathrm{MWd} /$ ton | $2.899010^{14}$ |  |  |  |  |  |  |  |
| 42,500 MWd/ton | $3.965210^{14}$ |  |  |  |  |  |  |  |
| $\sigma_{\text {fission }}\left({ }_{92}^{235} U\right)$ [barn] | 1 |  | 2 |  | 3 |  | 4 |  |
| $0 \mathrm{MWd} /$ /on | 1.2166 |  | 1.8537 |  | 27.130 |  | 270.96 |  |
| 42,500 MWd/ton | 1.2173 |  | 1.8804 |  | 27.099 |  | 281.54 |  |

$$
\sigma_{\max w}\left({ }_{92}^{235} U\right)=\sigma_{0}\left({ }_{92}^{235} U\right) \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}=368.06 \mathrm{barns}
$$

Table 7.6 gives the flux values for 1,2 and 4 groups and the fission cross sections of ${ }_{92}^{235} U$ at 4 energy groups:

At 0 MWd/ton: $\frac{\Phi_{\text {th }}}{\Phi_{\text {total }}}=\frac{\sigma_{\text {apollo }}\left({ }_{92}^{235} U\right)}{\sigma_{0}\left({ }_{92}^{235} U\right) \cdot \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}} \frac{\Phi_{4}}{\sum_{g=1,4} \Phi_{g}}=\frac{270.96}{368.06} \frac{0.36662 \times 10^{14}}{2.8995 \times 10^{14}}=0.093$
At 42, $500 \mathrm{MWd} /$ ton: $\frac{\Phi_{\text {th }}}{\Phi_{\text {total }}}=\frac{\sigma_{\text {apollo }}\left({ }_{92}^{235} U\right)}{\sigma_{0}\left({ }_{92}^{235} U\right) \cdot \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}} \frac{\Phi_{4}}{\sum_{g=1,4} \Phi_{g}}=\frac{281.54}{368.06} \frac{0.4571 \times 10^{14}}{3.9652 \times 10^{14}}=0.088$

The Maxwell thermal flux is worth slightly less than $10 \%$ of the total flux. The epithermal flux spectrum $r$ is obtained using the formula:

$$
r=\frac{\Phi_{e p i}}{\Phi_{t h}}=\frac{E \Phi(E)}{\Phi_{t h}}
$$

where $E \Phi(E)$ is the flux per unit of lethargy in epithermal macro-group 3 of APOLLO-calculated by dividing the integrated flux in this group by the difference in lethargy. $\Phi_{t h}$ is the Maxwell-distributed flux. The flux is integrated over macro-group 3 (epithermal) to calculate $\Phi_{e p i}$.

$$
\begin{aligned}
\Phi_{3} & =\int_{\text {group } 3} \Phi(E) d E \\
& =\int_{\text {group } 3}\left(\Phi_{\text {thermal }} \frac{E}{(k T)^{2}} e^{-\frac{E}{k T}}+\Phi_{\text {thermal }} \frac{\sqrt{\pi}}{2} \frac{\Sigma_{a}(k T)}{\xi \Sigma_{S}-\Sigma_{a}(k T)} \frac{\Delta(E /(k T))}{E}\right) d E
\end{aligned}
$$

The thermal component is equal to 0 in the epithermal group, where:

$$
\Phi_{3}=\int_{\text {group } 3} \Phi(E) d E=\int_{\text {group } 3} \Phi_{\text {epi }} \frac{\Delta(E /(k T))}{E} d E
$$

In macro-group $3, \Delta(E /(k T))=1$, hence: $\Phi_{3}=\int_{\text {group } 3} \Phi(E) d E=\Phi_{\text {ep } i}$ $\int_{\text {group } 3} \frac{1}{E} d E \Phi_{\text {epi }} \Delta u_{3}$

Finally, $r=\frac{\Phi_{\text {epi }}}{\Phi_{t h}}=\frac{\frac{\Phi_{3}}{\Delta u_{3}}}{\Phi_{4} \frac{\sigma_{4}^{\text {fission }}\left(\begin{array}{c}235 \\ 92\end{array}\right.}{\sigma_{0}^{\text {fission }}\binom{235}{92} \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}}}=\frac{\left.\Phi_{3} \sigma_{0}^{\text {fission }}\left(\begin{array}{c}235 \\ 92\end{array}\right]\right) \frac{\sqrt{\pi}}{2} \sqrt{T_{0} / T}}{\Delta u_{3} \Phi_{4} \sigma_{4}^{\text {fission }}\left({ }_{92}^{235} U\right)}$

$$
\left\{\begin{array}{l}
r=\frac{0.542910^{14} .368 .06}{(16.588-8.4) 0.366210^{14} 270.96}=0.291 \quad \text { at } 0 \mathrm{MWd} / \mathrm{ton} \\
r=\frac{0.930910^{14} .368 .06}{(16.588-8.4) \quad 0.457110^{14} 281.54}=0.325 \quad \text { at } 42,500 \mathrm{MWd} / \mathrm{ton}
\end{array}\right.
$$

This method enables calculation of capture rates of fission products with sufficient precision for engineering applications.

## Chapter 8 <br> The Boltzmann Equation

In 1879, Ludwig Boltzmann established the equation governing the behavior of particles in a gas of molecules, without interaction except for collisions between the said molecules. A parallel can in fact be drawn between the behavior of neutrons in matter and that of a ideal gas whose molecules would "disappear" as a result of some collisions, similar to what happens in some chemical reactions. Under this assumption, it is indeed the Boltzmann equation that governs the behavior of neutrons.

### 8.1 Setting Up the Boltzmann Equation

(Barjon 1993; Bellman et al. 1969; Blaquière 1962; Bussac and Reuss 1985; Case et al. 1953; Davison 1957; Duderstadt and Hamilton 1976; Duderstadt and Martin 1979; Lewis and Miller 1993; Tait 1964; Weinberg and Wigner 1958; Wing 1962)

The equation governing the behavior of the molecules of a free gas was established by Ludwig Boltzmann ${ }^{1}$ (1844-1906) in 1879 (Photo 8.1). His

[^136]
## Photo 8.1 Ludwig

Boltzmann (1844-1906)
(Public domain)

substantial works in statistical physics and thermodynamics had a deep impact on modern science. He showed that, statistically, the states of matter with the highest entropy were the most likely, on a large scale. Hence, a gas contained in a halfvolume separated by a partition from another empty half-volume, would always spread into the empty half-volume if the partition was removed, giving sense to the aphorism of Aristotle "Nature abhors a vacuum". The inverse case of a gas containing itself "on its own" in a smaller volume is impossible, whereas at the microscopic scale, all phenomena are reversible (Jeans 1925).

The neutron density in a reactor being very low, similar to a gas, a parallel can be drawn between the neutron scattering collisions on matter and the collisions between the molecules of a gas, while neglecting the very unlikely neutron-neutron collisions.

The application to neutrons and the standardization of the current notations owe much to the theoretical work developed within the framework of the Manhattan project (for the atomic bomb) at Los Alamos. This was between 1942 and 1945, particularly through the works (Photo 8.2) of K.M. Case, ${ }^{2}$

[^137]F. de Hoffmann ${ }^{3}$ and G. Placzek (whom we have already talked about). The 50's saw an important development in the methods of solving the Boltzmann equation, which were then explored in the 60's with the rise of computer science. Transport theory covers at the same times kinematic models in gases, transport of photons or neutrons or charged particles (including plasmas). It became common parlance in the scientific community to use the term transport for elementary particles such as the neutron, while the term radiative transfer is associated with photons and the terms kinetic theory or gas dynamics are applied for molecules (Photo 8.2).

In its most general form, the density of neutrons at a point in space depends on the neutron speed (which is equivalent to its energy), the direction $\vec{\Omega}$ of this speed, time and of course the point $\vec{r}$ of the considered space, $n(\vec{r}, v, \vec{\Omega}, t)$.


Kenneth Case (Public domain)
${ }^{3}$ Frederic de Hoffmann (1924-1989) is a physicist of Czech origin who immigrated to the USA in 1941 to complete his scientific studies at Harvard, then worked on the Manhattan project as from 1944. He assisted E. Teller at the beginning of the 50's on the Hydrogen bomb project. As from 1955, thanks to his management skills, he became the president of General Atomics, a company that builds reactors. He then redirected his career towards biomedical research by becoming the president of the Salt Institute in 1970. He died of AIDS which he contracted from an infected blood transfusion. His legacy includes important theoretical works in particle physics, where his name is often associated with that of H. Bethe.


Frederic de Hoffmann (Public domain)

# INTRODUCTION TO THE THEORY OF NEUTRON DIFFUSION 

Volume I



Photo 8.2 The work of Case, de Hoffmann and Placzek (1953) is a real cornerstone in the world of neutron transport: indeed, it is the first book published in this field. Its paper cover and glued binding are the reasons few copies survived to this day. However, there is no reactor physics department in the world that does not have at least one copy. A second volume was planned but never published (The Marguet collection)

### 8.1.1 Concept of Flux

(Mayo 1998, p119)
The angular flux is defined by:
Angular Flux: $\quad \Phi(\vec{r}, v, \vec{\Omega}, t) \equiv n(\vec{r}, v, \vec{\Omega}, t) v$

Fig. 8.1 Neutron flux density

$n(\vec{r}, v, \vec{\Omega}, t) d^{3} r d v d \Omega$ represents the number of neutrons at point $\vec{r}$ within an interval $d^{3} r$, having speed $v$ within an interval $d v$, going in the direction $\vec{\Omega}$ within a solid angle interval $d \Omega$, and at time $t$. This notion, by definition, is considered within a volume. Hence, the concept of angular flux is also based on a volume intensive property. In this approach, point particles are assumed and it can be easily imagined how the flux does not have any meaning below a certain scale because of neutron shape (Fig. 8.1).

The integral of the angular flux over $4 \pi$ steradians defines the flux spectrum at a point in space (here, in terms of the speed but the energy variable can also be used) (Baur 1985, p22),

$$
\begin{equation*}
\text { Flux spectrum: } \quad \Phi(\vec{r}, v, t) \equiv n(\vec{r}, v, t) \cdot v=\int_{4 \pi} \Phi(\vec{r}, v, \vec{\Omega}, t) d \Omega \tag{8.2}
\end{equation*}
$$

The flux $\Phi(\vec{r}, v, t)$ accounts for all the neutrons of speed $v$ (whichever their direction) which are found in the volume element $d^{3} r$. Its unit, the number of neutrons (of speed $v$ ) per $\mathrm{cm}^{2}$ per second might lead to believe that only the neutrons going through a given surface are counted. This is not true since all neutrons in the volume element contribute to the flux (Fig. 8.2).

It will be noted that such an approach is meaningful only for a sufficiently large volume compared to the volume occupied on average by a neutron ( $\approx 4.10^{-39} \mathrm{~cm}^{3}$ ). The angular flux $\Phi(\vec{r}, v, \vec{\Omega}, t)$ accounts only for the neutrons of speed $v$ going in the direction $\vec{\Omega}$. The angular neutron current is a vector quantity that depends on space, speed (or energy), direction and time in the transient regime (Baur 1985, p28):

$$
\begin{equation*}
\text { Angular neutron current: } \quad \vec{J}(\vec{r}, v, \vec{\Omega}, t) \equiv \vec{\Omega} \cdot \Phi(\vec{r}, v, \vec{\Omega}, t) \tag{8.3}
\end{equation*}
$$

It will be noted that the dimensions of the vector components of the neutron current are the same as that of a flux-from which stems a certain amount of confusion. If we consider a surface element $d S$ with a normal $\vec{n}$, the quantity

Fig. 8.2 Neutron flux


Fig. 8.3 Neutron current density

$\vec{J}(\vec{r}, v, \vec{\Omega}, t) \cdot \vec{n} d S d v$ is the number of neutrons with a speed $v$ within a $d v$ interval, that cross the surface $d S$ at time $t$ (Fig. 8.3).

If the surface element is perpendicular to the direction of motion of the monokinetic and mono-directional (in direction $\vec{\Omega}$ ) neutrons, i.e., if $\vec{n}=\vec{\Omega}$, the number of neutrons with speed $v$ within a $d v$ interval that crosses the surface is equal to $\Phi(\vec{r}, v, \vec{\Omega}, t) d S d v$. In this specific case, the notions of current and flux blur together. However, generally, the number of neutrons that cross the surface is given by $\Phi(\vec{r}, v, \vec{\Omega}, t) d S d v \vec{n} . \vec{\Omega}$. The net current is defined as the integral over all directions and all speeds of the current density:

$$
\text { Neutron current: } \begin{align*}
\vec{J}(\vec{r}, t) & =\int_{\Omega} d \Omega \int_{v} d v \vec{J}(\vec{r}, v, \vec{\Omega}, t)=\int_{\Omega} d \Omega \int_{v} d v \Phi(\vec{r}, v, \vec{\Omega}, t) \vec{\Omega} \\
& =\int_{\Omega} d \Omega \Phi(\vec{r}, \vec{\Omega}, t) \vec{\Omega} \tag{8.4}
\end{align*}
$$

The quantity $\vec{J}(\vec{r}, t) \cdot \vec{n} d S$ represents the number of neutrons that cross the surface element $d S$. Physically, this corresponds to a net current density (Goldstein 1959, p9). This is just called current in neutronics. It will be noted that neutrons

Fig. 8.4 Example of current and flux

whose velocity make an acute angle ( $\vec{v} \cdot \vec{n}>0$ ) with the normal are counted positively. Those which make an obtuse angle ( $\vec{v} \cdot \vec{n}<0$ ) are counted negatively, and counterbalance in the net current the neutrons going in the "positive" direction. Those that are perpendicular are not counted, since they do not really cross the surface. The concept of current and flux applies to particles other than neutrons, as well as other properties. Hence, the energy current density corresponds to the net energy that crosses a unit surface per unit time (Goldstein 1959, p9). This will be illustrated with a simple example. Consider the neutron balance in Fig. 8.4:

In this simple example, it is assumed that 3 neutrons per second cross the unit surface $d x d y$ along the positive $\vec{z}$ axis with the unit speed $v=1 \mathrm{~cm} / \mathrm{s}$, while one neutron per second crosses from top to bottom. In this case, the net current is 2 neutrons per $\mathrm{cm}^{2}$ per second. It can be seen that a positive partial scalar current, also called outgoing current, can be defined such that:

$$
J^{+}(\vec{r}, t)=\int_{\vec{\Omega} \cdot \vec{n}>0} \vec{J}(\vec{r}, t) \cdot \vec{n}
$$

which is equal to 3 neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$ in the given example. Similarly, a negative partial current, also called an incoming current, can be defined (Baur 1985, p30),

$$
J^{-}(\vec{r}, t)=\int_{\vec{\Omega} \cdot \vec{n}<0} \vec{J}(\vec{r}, t) \cdot \vec{n}
$$

which is equal to -1 neutros $/ \mathrm{cm}^{2} / \mathrm{s}$ in this example. This current is negative to the extent that it was defined with $\vec{n}=+\vec{z}$. The sum of the positive and negative currents yield the net current projected in the considered direction:

$$
\vec{J}(\vec{r}, t) \cdot \vec{z}=J^{+}(\vec{r}, t)+J^{-}(\vec{r}, t)
$$

With such an orientation of the normal, the negative current is always negative by construction, since only neutrons with $\vec{\Omega} \cdot \vec{n}<0$ are considered. Some authors
such as Kenneth Shultis ${ }^{4}$ and Richard Faw (Shultis and Faw 2000, p19), prefer using as negative current the absolute value of our definition (so as to deal with physically positive values), in which case the net current is obtained by the difference between the positive and negative currents. If we add to the given example a neutron per second that goes from left to right ( $\vec{v}=v \vec{y}$ ) and a neutron per second that goes from right to left $(\vec{v}=-v \vec{y})$, this does not change the net current across the surface $d x d y$ but these neutrons will contribute to the flux which will be 6 neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$. The net current in the $\vec{y}$ direction is zero since the positive and negative currents along this axis are equal in magnitude ( 1 neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$ ), and cancel each other out. Since there are no neutrons along the $\vec{x}$-axis, both partial and net currents are zero along that axis. Hence, the current components, in our example, are:

$$
\vec{J}(\vec{r})=\left(\begin{array}{c}
0 \\
0 \\
2
\end{array}\right) \quad \vec{J}^{+}(\vec{r})=\left(\begin{array}{c}
0 \\
1 \\
3
\end{array}\right) \quad \vec{J}^{-}(\vec{r})=\left(\begin{array}{c}
0 \\
-1 \\
-1
\end{array}\right)
$$

It is important to note the bottom-line here: the absence of a net current in a direction does not necessarily mean that there are no neutrons moving in that direction. At most, it can be said that there are as many neutrons moving in that direction, as there are moving in the opposite direction. In particular, in the case of a $1 D$ geometry (for example $\vec{x}$ ), one should be careful to note that neutrons do travel in the $\vec{y}$ and $\vec{z}$ directions but in equal amounts (Fig. 8.5).

An isotropic flux corresponds to an angular neutron density independent of direction $\vec{\Omega}$ and is given by:

[^138]
(courtesy Shultis)

Fig. 8.5 Real symmetric trajectories of neutrons in a $1 D$ geometry along $x$


Isotropic flux: $\quad \Phi(\vec{r}, v, \vec{\Omega}, t)=\frac{1}{4 \pi} \Phi(\vec{r}, v, t)$,
where the integration over $4 \pi$ steradians is trivial.
In its most general form, the Boltzmann equation depends on 7 variables: the 3 spatial coordinates, the 3 velocity coordinates and time. It should be noted, however, regarding the velocity variable, that it is more conventional to use the two angular variables for the direction vector $\vec{\Omega}$ of the particle, and the magnitude $v$ of the velocity, or the kinetic energy $E=m v^{2} / 2$ of the particle. The reason for this approach is that the macroscopic cross sections do not depend on $\vec{\Omega}$ in isotropic materials but do depend on $v$. In the case of an isotropic flux, the positive current can be calculated by integration over the angular directions oriented in the positive half space, where $\vec{n}$ is the normal pointing inwards:

$$
\begin{aligned}
J^{+}(\vec{r}, v, t) & =\int_{\vec{\Omega} \cdot \vec{n}>0} \Phi(\vec{r}, v, \vec{\Omega}, t) \vec{\Omega}, \vec{n} d \vec{\Omega}=\frac{1}{4 \pi} \Phi(\vec{r}, v, t) \int_{\vec{\Omega} \cdot \vec{n}>0} \vec{\Omega} \cdot \vec{n} d \vec{\Omega} \\
& =\frac{1}{4 \pi} \Phi(\vec{r}, v, t) \int_{0}^{\frac{\pi}{2}} \cos \theta 2 \pi \sin \theta \mathrm{~d} \theta=\frac{\Phi(\vec{r}, v, t)}{4}
\end{aligned}
$$

A similar calculation for the negative current yields:

$$
J^{-}(\vec{r}, v, t)=\int_{\vec{\Omega} \cdot \vec{n}>0} \Phi(\vec{r}, v, \vec{\Omega}, t) \mathrm{d} \vec{\Omega}=-\frac{\Phi(\vec{r}, v, t)}{4}
$$

which, in this case, translates to a net zero current. Note that for any plane going through $\vec{r}$, the positive current at that point is $\Phi(\vec{r}, v, t) / 4$, while the negative current
is $-\Phi(\vec{r}, v, t) / 4$. But this result is valid only for isotropic fluxes. Physically, this is very much questionable, as for example at the interface between two different media, but this equivalence will still be used in later sections.

### 8.2 The Integro-Differential Transport Equation

### 8.2.1 The Integro-Differential Transport Equation in Kinetics

If a neutron balance is done on a reactor volume element, we have to consider on one hand the neutron production, either by neutron sources or by slowing-down of neutrons (or acceleration in the thermalization zone), and on the other hand, terms accounting for streaming-out and leakage:

Differential form of the Boltzmann equation:

$$
\begin{align*}
& \frac{\partial n(\vec{r}, v, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, v, \vec{\Omega}, t)+\Sigma_{t}(\vec{r}, v, \vec{\Omega}, t) \Phi(\vec{r}, v, \vec{\Omega}, t) \\
= & S(\vec{r}, v, \vec{\Omega}, t)+\int_{0}^{\infty} d v^{\prime} \int_{4 \pi} d \Omega^{\prime} \Sigma_{S}\left(\vec{r}, v^{\prime} \rightarrow v, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, t\right) \Phi(\vec{r}, v, \vec{\Omega}, t) \tag{8.6}
\end{align*}
$$

The flux is introduced in the time derivative through $n(\vec{r}, v, \vec{\Omega}, \mathrm{t})=$ $\Phi(\overrightarrow{\mathrm{r}}, v, \vec{\Omega}, \mathrm{t}) / v$. Of note here is that the speed is time-independent since the neutron population of a given speed $v$ is considered. This is the integro-differential form of the linear Boltzmann equation, with integrations over energy and angle, and space and time derivatives. Also the equation here is termed linear compared to the original Boltzmann equation for gases since the latter contains a quadratic term in number of particles. This quadratic term arises from the scattering collisions of particles onto one another, but is negligible in the approximation of "low $n$ ", e.g. few neutrons in the reactor. This approximation here implies that the density of neutrons is not significant compared to the density of the target nuclei, and is low enough to ignore neutron-neutron collisions. These two assumptions are very much satisfied in reactor physics (Reed and Simon 1979, p245). In writing the equation, ${ }^{5}$ external forces such as gravity were ignored, because of the very low mass of the neutron and their small mean lifetime. Radioactivity is also neglected since the free

[^139]neutron half-life is much longer than, again, the mean lifetime. Moreover, the collisions are assumed to be between point particles. Indeed, if we consider the radii of the interacting particles and an interaction governed by a potential well, it is the Enskog equation that should be used-and this is beyond the scope of this text. The slowing down operator $R[]=\int_{0}^{\infty} d v^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, v^{\prime} \rightarrow v, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, t\right)[]$ is sometimes called the kernel of the transport equation, analogous to integral equations (Jerri 1999, p3). In the previous equation, the speed variable was used to characterize the neutron population but the energy variable can also be used:
\[

$$
\begin{aligned}
& \frac{1}{\sqrt{\frac{2 E}{m}}} \frac{\partial \Phi(\vec{r}, E, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \mathrm{E}, \vec{\Omega}, t)+\Sigma_{t}(\vec{r}, E, \vec{\Omega}, t) \Phi(\vec{r}, E, \vec{\Omega}, t) \\
& =S(\vec{r}, E, \vec{\Omega}, t)+\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, t\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}, t\right)
\end{aligned}
$$
\]

The identity below was used:

$$
\operatorname{div}(\vec{J})=\operatorname{div}(\vec{\Omega} \Phi)=\vec{\Omega} \cdot \overrightarrow{\operatorname{grad} \Phi}+\underbrace{\Phi \operatorname{div} \vec{\Omega}}_{0}
$$

which allows the leakage term to be expressed either in the form $\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi$ $(\vec{r}, v, \vec{\Omega}, t)$ or $\operatorname{div}(\vec{\Omega} \cdot \Phi(\vec{r}, v, \vec{\Omega}, t))$. In this approach, $\vec{\Omega}$ is a constant since the Boltzmann equation is written for a given direction $\vec{\Omega}$ and a given speed $v$. In the case of fission, the source can be regarded as being isotropic (i.e. independent of $\vec{\Omega}$ ). The fission source is then made up of two terms: the prompt fission term given by the fission spectrum $\chi_{\text {prompt }}(E)$, and the delayed neutrons ( $P$ groups of Precursors of concentration $C_{i}$ and decay constant $\lambda_{i}$-in general, 6 groups) given by the spectrum $\chi_{\text {delayed } i}(E)$, which depends on energy, or even on the delayed neutron group, denoted here by $i$.

Isotropic fission source : $S(\vec{r}, E, t)$

$$
\begin{equation*}
=\frac{1}{4 \pi}\left(\chi_{\text {prompt }}(E) \int_{4 \pi} d \Omega^{\prime} \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(\vec{r}, E^{\prime}, t\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}, t\right)+\sum_{i=1}^{P} \lambda_{i} C_{i}(\vec{r}, t) \chi_{\text {delayed }_{i}}(E)\right) \tag{8.7}
\end{equation*}
$$

### 8.2.2 The Integro-Differential Equation in Steady-State

### 8.2.2.1 Setting Up the Integro-Differential Form

In steady state, the $\partial n(\vec{r}, E, \vec{\Omega}, t) / \partial t$ term disappears. The Boltzmann equation is then conventionally written in the form:

$$
\begin{aligned}
\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, E, \vec{\Omega})+\Sigma_{t}(\vec{r}, E, \vec{\Omega}) \Phi(\vec{r}, E, \vec{\Omega})= & \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \\
& \times \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)+S(\vec{r}, E, \vec{\Omega})
\end{aligned}
$$

The integration over angle of the Boltzmann equation in steady state is then given by:

$$
\begin{aligned}
& \int_{4 \pi} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E, \vec{\Omega}) d \Omega+\int_{4 \pi} \Sigma_{t}(\vec{r}, E, \vec{\Omega}) \Phi(\vec{r}, E, \vec{\Omega}) d \Omega \\
& \quad-\int_{4 \pi} d \Omega \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \Omega \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)=\int_{4 \pi} S(\vec{r}, E, \vec{\Omega}) d \Omega
\end{aligned}
$$

Using the identity $\operatorname{div}(\vec{\Omega} \Phi)=\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi$, the first term can be expressed as:

$$
\begin{aligned}
\int_{4 \pi} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E, \vec{\Omega}) d \Omega & =\int_{4 \pi} \operatorname{div}(\vec{\Omega} \cdot \Phi(\vec{r}, E, \vec{\Omega})) d \Omega \\
& =\operatorname{div}\left(\int_{4 \pi}(\vec{\Omega} \cdot \Phi(\vec{r}, E, \vec{\Omega})) d \Omega\right)=\operatorname{div}(\vec{J}(\vec{r}, E))
\end{aligned}
$$

with the usual definition of the current:
Neutron current: $\quad \vec{J}(\vec{r}, E) \equiv \int_{4 \pi} \vec{J}(\vec{r}, E, \vec{\Omega}) d \Omega=\int_{4 \pi} \vec{\Omega} . \Phi(\vec{r}, E, \vec{\Omega}) d \Omega$
Assuming that the total cross section is isotropic, the second term simplifies to:

$$
\int_{4 \pi} \Sigma_{t}(\vec{r}, E, \vec{\Omega}) \Phi(\vec{r}, E, \vec{\Omega}) d \Omega=\Sigma_{t}(\vec{r}, E) \int_{4 \pi} \Phi(\vec{r}, E, \vec{\Omega}) d \Omega=\Sigma_{t}(\vec{r}, E) \Phi(\vec{r}, E)
$$

The third term involves the usual assumption that the doubly-differential scattering cross section $\Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right)$ is in fact only a function of the scalar product $\vec{\Omega}^{\prime} \cdot \vec{\Omega}$, the directions before and after the collision, i.e., the cosine of the angle between these directions, conventionally denoted by $\mu$ (Fig. 8.6).

$$
\Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right)=\Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} . \vec{\Omega}\right)=\Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \mu\right)
$$

This dependence of the differential scattering cross section on the scalar product $\vec{\Omega}^{\prime} \cdot \vec{\Omega}$ is nearly always true, except in crystalline media, where the bonds introduce anisotropy in the problem. However, the error due to this assumption is small, leading to:

Fig. 8.6 Spherical coordinates


$$
\begin{aligned}
& \int_{4 \pi} d \Omega \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \Omega^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime} \vec{\Omega}^{\prime}\right) \\
& \quad=\int_{4 \pi} d \Omega^{\prime} \Phi\left(\vec{r}, E^{\prime} \vec{\Omega}^{\prime}\right) \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \Omega \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} . \vec{\Omega}\right)
\end{aligned}
$$

Using the differential solid angle in spherical coordinates, ${ }^{6} d \Omega=\sin \theta d \theta d \varphi$, then performing the following change of variable, $\mu=\cos \theta, d \mu=-\sin \theta d \theta$, in the above integral, the following is obtained:

$$
\begin{aligned}
\int_{4 \pi} d \Omega \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} . \vec{\Omega}\right) & =\int_{2 \pi} d \varphi \int_{0}^{\pi} d \theta \sin \theta \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \mu\right) \\
& =2 \pi \int_{-1}^{+1} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \mu\right) d \mu
\end{aligned}
$$

Finally, using simplified notations for the scattering cross section and the flux as function of energy, the scattering cross section is written:

$$
\Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E\right)=2 \pi \int_{-1}^{+1} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \mu\right) d \mu \quad \text { and } \quad \Phi\left(\vec{r}, E^{\prime}\right)=\int_{4 \pi} \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) d \Omega^{\prime}
$$

The term accounting for neutrons scattering in the considered volume element can be simplified to:

[^140]\[

$$
\begin{aligned}
& \int_{4 \pi} d \Omega \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \Omega^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) \\
& =\int_{4 \pi} \int_{0}^{\infty} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) d \Omega^{\prime} d E^{\prime}=\int_{0}^{\infty} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}
\end{aligned}
$$
\]

The fission source term without delayed neutrons, generally considered isotropic, is written as the integral of the number of neutrons produced, integrated over all energies and angles:

$$
\begin{aligned}
\int_{4 \pi} S(\vec{r}, E, \vec{\Omega}) d \Omega & =\frac{\chi_{\text {prompt }}(E)}{4 \pi} \int_{4 \pi} d \Omega \int_{4 \pi} d \Omega^{\prime} \int_{0}^{\infty} d E^{\prime} v \Sigma_{f}\left(\vec{r}, E^{\prime}\right) \Phi\left(\vec{r}, E^{\prime}, \overrightarrow{\Omega^{\prime}}\right) \\
& =\chi_{\text {prompt }}(E) \int_{4 \pi}^{\infty} \int_{0}^{\infty} d E^{\prime} v \Sigma_{f}\left(\vec{r}, E^{\prime}\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}\right) d \Omega^{\prime} \\
& =\chi_{\text {prompt }}(E) \int_{0}^{\infty} d E^{\prime} v \Sigma_{f}\left(\vec{r}, E^{\prime}\right) \Phi\left(\vec{r}, E^{\prime}\right)
\end{aligned}
$$

Bringing together the four terms that have been calculated so far leads to what is known as the integro-differential form of the Boltzmann transport equation. This equation relates the flux spectrum and the spatial derivative of the neutron current:

Steady-state integro-differential form of the Boltzmann equation:

$$
\begin{align*}
\operatorname{div}(\vec{J}(\vec{r}, E))+\Sigma_{t}(\vec{r}, E) \Phi(\vec{r}, E)= & \int_{0}^{\infty} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}  \tag{8.9}\\
& +\chi_{\text {prompt }}(E) \int_{0}^{\infty} d E^{\prime} v \Sigma_{f}\left(\vec{r}, E^{\prime}, t\right) \Phi\left(\vec{r}, E^{\prime}\right)
\end{align*}
$$

It is common practice to simplify notation by introducing a transport operator $T$ such that, in transient states:

$$
\begin{aligned}
& \underbrace{\left\{\frac{1}{v} \frac{\partial}{\partial t}+\Sigma_{t}(\vec{r}, E, \vec{\Omega}, t)+\vec{\Omega} \cdot \overrightarrow{g r a d}\right\}}_{T_{T]}}[\Phi(\vec{r}, E, \vec{\Omega}, t)] \\
& =\underbrace{\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \Omega^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime}\right.}_{\underbrace{R[\Phi(\vec{r},, \overrightarrow{,}, t)]}} \rightarrow \vec{\Omega}, t) \Phi\left(\vec{r}, E, \vec{\Omega}^{\prime}, t\right) \\
& +\underbrace{S(\vec{r}, E, \vec{\Omega}, t)}_{\begin{array}{c}
\text { Non fissision neurron source } \\
\text { in the ovlume }
\end{array}}+\underbrace{\chi \nu \Sigma_{f} \Phi(\vec{r}, E, \vec{\Omega}, t)}_{\text {fision sources }}
\end{aligned}
$$

The source terms on the right hand side of the equation comprise the slowingdown sources represented by the slowing down operator $R[\Phi(\vec{r}, E, \vec{\Omega}, t)]$, sources independent of the flux $S(\vec{r}, E, \vec{\Omega}, t)$ (also called not-coupled-to-the-flux sources or external sources such as startup point-wise sources, inherent sources of spontaneous fission or ( $\alpha, n$ ) sources), and the fission sources represented in a mnemonic way by the following term, often isotropic:

$$
\begin{aligned}
\chi \nu \Sigma_{f} \Phi(\vec{r}, E, \vec{\Omega}, t) & =\chi(\vec{r}, E) v(\vec{r}, E, t) \Sigma_{f}(\vec{r}, E, \vec{\Omega}, t) \Phi(\vec{r}, E, \vec{\Omega}, t) \\
& =\frac{\chi(\vec{r}, E) v(\vec{r}, E, t) \Sigma_{f}(\vec{r}, E, t)}{4 \pi} \Phi(\vec{r}, E, \vec{\Omega}, t)
\end{aligned}
$$

In steady-state and in the absence of external sources, the source term is proportional to the flux, giving rise to the equation:

$$
[T-R][\Phi(\vec{r}, E, \vec{\Omega})]=\chi \nu \Sigma_{f} \Phi(\vec{r}, E, \vec{\Omega})
$$

It can be mathematically shown (Planchard 1995) that the operator $[T-R]^{-1}$ is positive over the $L^{2}(\vec{\Omega} \times R)$ space, and non-negative with respect to the scalar energies $E$.

### 8.2.2.2 The Eigenvalue Problem

The critical reactor problem with one energy group ${ }^{7}$ is written, using the above notations, like any eigenvalue problem (Wilkinson 1965):

$$
[T-R][\Phi(\vec{r}, \vec{\Omega})]=\frac{\chi v \Sigma_{f} \Phi(\vec{r}, \vec{\Omega})}{k_{e f f}}
$$

Using the inverse operator,

$$
[T-R]^{-1}\left[\chi \nu \Sigma_{f} \Phi(\vec{r}, \vec{\Omega})\right]=k_{e f f} \Phi(\vec{r}, \vec{\Omega})
$$

In kinetics, the source term is more complex because it couples with the delayed neutrons. Generally, an overall operator $H=T-R$ is also used such that:

$$
\begin{equation*}
H[\Phi(\vec{r}, \vec{\Omega})]=\frac{\chi v \Sigma_{f} \Phi(\vec{r}, \vec{\Omega})}{k_{e f f}} \tag{8.10}
\end{equation*}
$$

[^141]It can be shown here that the operator $[H]^{-1} \chi v \Sigma_{f}$ allows for a unique positive eigenvector $\Phi_{0}$ with a positive eigenvalue $\lambda_{0}$ equal to the spectral radius of the matrix of the operator $[H]^{-1} \chi v \Sigma_{f}$ (Jentzsch theorem). This eigenvalue is called the $k$ effective and the physical importance of this mathematical concept will be thoroughly discussed in Chap. 11. All the other eigenvalues are smaller in magnitude to $\lambda_{0}$, and tend to 0 . J. Planchard points out that in the multi-group case, it is likely that the other eigenvalues are real and positive, even if there does not exist a rigorous mathematical demonstration of the fact. However, it is what happens in the neutronics case with physical values. This property ensures the convergence of the power iteration method, which will be discussed in the chapter on diffusion. Also, dividing the neutron production terms by $k_{\text {eff }}$ is arbitrary, and several formulations of the eigenvalue reactor problem ${ }^{8}$ exist.

$$
\begin{aligned}
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})= & \frac{v \Sigma_{f}(\vec{r})}{k_{e f f}} \int_{\vec{\Omega}} d \vec{\Omega} \Phi(\vec{r}, \vec{\Omega}) \\
& +\int_{\vec{\Omega}} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)+S(\vec{r}, \vec{\Omega})
\end{aligned}
$$

is called the $k_{\text {eff }}$ formulation of the criticality equation, and it will be very much used in this text.

$$
\begin{aligned}
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})= & \lambda \Phi(\vec{r}, \vec{\Omega})+v \Sigma_{t}(\vec{r}) \int_{\vec{\Omega}} d \vec{\Omega} \Phi(\vec{r}, \vec{\Omega}) \\
& +\int_{\vec{\Omega}^{\prime}} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)+S(\vec{r}, \vec{\Omega})
\end{aligned}
$$

is called the $\lambda$ formulation, and is more adapted to a time-dependent problem of a (burst) Dirac source introduced in the system ( $\lambda$ is sometimes called the timeeigenvalue), while:
$\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})$

$$
=c\left[v \Sigma_{f}(\vec{r}) \int_{\vec{\Omega}} d \vec{\Omega} \Phi(\vec{r}, \vec{\Omega})+\int_{\vec{\Omega}} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)\right]+S(\vec{r}, \vec{\Omega})
$$

[^142]is called the $c^{9}$ formulation. Choosing which formulation of the eigenvalue equation to use is important as the set of the eigenvalues from each of these three formulations is different. Also, the eigenvectors which can be either discrete or continuous are not interchangeable from one problem formulation to another. Finally, one equation can have complex eigenvalues (such as the equation in $c$ ) while another can have all its eigenvalues real (such as the equation in $k_{\text {eff }}$. Regarding the $k_{\text {eff }}$ problem, a Green's function $G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)$ can be introduced and is defined by:
\[

$$
\begin{aligned}
& \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)+\Sigma_{t}(\vec{r}) G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right) \\
&-\int_{\vec{\Omega}} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)=\delta\left(\vec{r}, \vec{r}_{0}\right) \delta\left(\vec{\Omega}, \vec{\Omega}_{0}\right)
\end{aligned}
$$
\]

i.e., the flux produced by a unit source placed at $\vec{r}_{0}$ in the $\vec{\Omega}_{0}$ direction. For solely the monoenergetic case, the reciprocity theorem for Green's functions can be used, which states that:

$$
G\left(\vec{r}, \vec{r}^{\prime}, \vec{\Omega}, \vec{\Omega}^{\prime}\right)=G\left(\vec{r}^{\prime}, \vec{r},-\vec{\Omega}^{\prime},-\vec{\Omega}\right)
$$

If reflective boundary conditions are used, the incoming flux at a point $\vec{r}_{s}$ of the surface is written:

$$
\Phi\left(\vec{r}_{S}, \vec{\Omega}\right)=\int_{\partial V} d^{2} r \int_{\vec{\Omega}^{\prime} \cdot \vec{n}^{\prime}>0} d \vec{\Omega}^{\prime} R\left(\vec{r}_{s},-\vec{\Omega}, \vec{r}_{s}^{\prime}, \vec{\Omega}^{\prime}\right) \vec{\Omega}^{\prime} \cdot \vec{n}^{\prime} \Phi\left(\vec{r}_{s}^{\prime}, \vec{\Omega}^{\prime}\right)
$$

where $\vec{n}^{\prime}$ is the normal to point $\vec{n}_{s}^{\prime}$, at the surface $\partial V$ of volume $V$. $R\left(\vec{r}_{s},-\vec{\Omega}, \vec{r}_{s}^{\prime} \vec{\Omega}^{\prime}\right)$ is the reflection coefficient which is usually a symmetric function with respect to its arguments:

$$
R\left(\vec{r}_{s},-\vec{\Omega}, \vec{r}_{s}^{\prime}, \vec{\Omega}^{\prime}\right)=R\left(\vec{r}_{s}^{\prime},-\vec{\Omega}^{\prime}, \vec{r}_{s}, \vec{\Omega}\right)
$$

The integral form involves calculating the flux as a solution in terms of Green's functions of the fission sources in the whole volume and of the surface sources:

$$
\begin{aligned}
& \Phi(\vec{r}, \vec{\Omega})=\int_{V} d^{3} r^{\prime} \int_{\vec{\Omega}^{\prime}} d \vec{\Omega}^{\prime} \frac{v \Sigma_{f}\left(\vec{r}^{\prime}\right)}{k_{e f f}} G\left(\vec{r}, \vec{r}^{\prime}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) \Phi\left(\vec{r}^{\prime}\right) \\
& +\int_{\partial V} d^{2} r_{s}^{\prime \prime} \int_{\partial V} d^{2} r_{s}^{\prime} \int_{\vec{\Omega}^{\prime} \cdot \vec{n}^{\prime}>0} d \vec{\Omega}^{\prime} \vec{\Omega}^{\prime} \cdot \vec{n}^{\prime} \int_{\vec{\Omega}^{\prime \prime} \cdot \vec{n}^{\prime \prime}>0} d \vec{\Omega}^{\prime \prime} \vec{\Omega}^{\prime \prime} \cdot \vec{n}^{\prime \prime} R\left(\vec{r}_{s}^{\prime},-\vec{\Omega}^{\prime}, \vec{r}_{s}^{\prime \prime}, \vec{\Omega}^{\prime \prime}\right) \\
& \quad\left[\Phi\left(\vec{r}_{s}^{\prime \prime}, \vec{\Omega}^{\prime \prime}\right) G\left(\vec{r}, \vec{\Omega}, \vec{r}_{s}^{\prime},-\vec{\Omega}^{\prime}\right)-\Phi\left(\vec{r}_{s}^{\prime}, \vec{\Omega}^{\prime}\right) G\left(\vec{r}, \vec{r}_{s}^{\prime \prime}, \vec{\Omega}, \vec{\Omega}^{\prime \prime}\right)\right]
\end{aligned}
$$

[^143]Owing to the properties of Green's functions, and of the angular flux on the surface, the term on the right hand side disappears, allowing the flux to be written as:

$$
\begin{aligned}
\Psi(\vec{r}) & \equiv \sqrt{v \Sigma_{f}(\vec{r})} \Phi(\vec{r}) \\
& =\frac{1}{k_{e f f}} \int_{V} \sqrt{v \Sigma_{f}(\vec{r})} \sqrt{v \Sigma_{f}\left(\vec{r}^{\prime}\right)} \underbrace{\sqrt{v \Sigma_{f}\left(\vec{r}^{\prime}\right)} \Phi\left(\vec{r}^{\prime}\right)}_{\psi\left(\vec{r}^{\prime}\right)} d^{3} r^{\prime} \int d \vec{\Omega} d \vec{\Omega}^{\prime} G\left(\vec{r}, \vec{r}^{\prime}, \vec{\Omega}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

The somewhat arbitrary introduction of the square root terms allows the impact of the real and symmetric integral operator to be clearly shown. This is a HilbertSchmidt type of operator, whose real eigenvalues are known to form a countable infinite set, with the origin being the only accumulation point.

$$
\Psi(\vec{r})=\frac{1}{k_{\text {eff }}} S H_{\vec{r}, \vec{r}^{\prime}}\left[\Psi\left(\vec{r}^{\prime}\right)\right]
$$

Also, it is known that there is no general eigenvector. Since this eigenvalue problem deals with the flux integrated over angle, Sahni points out that it has far fewer eigenvalues than the $c$ formulation of the same problem-hence its appeal.

### 8.2.2 3 Solutions of the Transport Equation for Simple Cases

In an infinite medium where the source is strictly proportional to the absorption cross section, the relation below is true:

$$
S(\vec{r})=\alpha \Sigma_{a}(\vec{r}) .
$$

The uniform and isotropic angular flux $\Phi(\vec{r}, \vec{\Omega})=\alpha /(4 \pi)$ is the trivial solution to the Boltzmann equation, since after integration over angle and energy, it simplifies to:

$$
\Sigma_{t}(\vec{r}) \Phi(\vec{r})=\alpha \Sigma_{s}(\vec{r})+\alpha \Sigma_{a}(\vec{r})
$$

where $\Phi(\vec{r})=\int_{4 \pi} \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}=\alpha$.
If the steady-state energy equation is integrated over energy, the monoenergetic integro-differential form of the transport equation is obtained:

$$
\begin{aligned}
& \vec{\Omega} . \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega}) \\
& =\int_{0}^{\infty} d E \int_{0}^{\infty} d E^{\prime} \int_{\vec{\Omega}^{\prime}} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)+S(\vec{r}, \vec{\Omega})
\end{aligned}
$$

The $\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})$ term corresponds to the derivative along the neutron path, in the direction $\vec{\Omega}$. In the very particular case where neutrons are considered in vacuum, the equation simplifies to:

Integro-differential form of the equation in vacuum:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})
$$

$$
\begin{equation*}
=\frac{\partial \Phi(\vec{r}, \vec{\Omega})}{\partial \ell}=S(\vec{r}, \vec{\Omega}) \tag{8.11}
\end{equation*}
$$

where $\ell$ is the coordinate ${ }^{10}$ depending on the direction $\vec{\Omega}$. Intuitively, the solution to Eq. 8.11 is given by:

$$
\Phi(\vec{r}, \vec{\Omega})=\int_{0}^{\infty} S(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}) d \ell
$$

which represents the fact that the flux is obtained by summing the contributions from the sources emitting in the $\vec{\Omega}$-direction before the point $\vec{r}$ (no collision in vacuum can deviate the neutrons). This result can also be obtained by rewriting Eq. 8.11 as:

$$
\frac{\partial \Phi(\vec{r}-\ell \vec{\Omega}, \vec{\Omega})}{\partial \ell}=S(\vec{r}-\ell \vec{\Omega}, \vec{\Omega})
$$

and integrating between $\ell=0$ and $\ell=\infty$. It is then assumed that the angular flux in the $\vec{\Omega}$-direction is zero at infinity, which is indeed the case of an isotropic point source $S$ (in neutron/s), whose angular flux in vacuum is $S /\left(4 \pi \ell^{2}\right)$. Only sources placed on the $\vec{\Omega}$ axis before $\vec{r}$ contribute to the angular flux in the same direction. Sources placed after $\vec{r}$ contribute to the flux in the $-\vec{\Omega}$ direction:

$$
\Phi(\vec{r},-\vec{\Omega})=\int_{0}^{\infty} S(\vec{r}+\ell \vec{\Omega},-\vec{\Omega}) d \ell
$$

If the completely hypothetical case of a purely absorbing medium (therefore non-scattering) is considered, the integro-differential equation is written as (Fig. 8.7):

[^144]

Fig. 8.7 Neutron transport in vacuum

Integro-differential form of the transport equation in an absorbing medium:

$$
\begin{equation*}
\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{a}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})=S(\vec{r}, \vec{\Omega}) \tag{8.12}
\end{equation*}
$$

The solution is obtained by adding an attenuation term to the previous solution for the vacuum case

Solution for the flux in an absorbing medium: $\Phi(\vec{r}, \vec{\Omega})=\int_{0}^{\infty} e^{-\overline{\Sigma_{a} \ell}} S(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}) d \ell$
where $e^{-\overline{\Sigma_{a} \ell}}$ is the exponential of the optical path, which is defined as ${ }^{11}$ :
Optical path in a purely absorbing medium: $\quad \overline{\Sigma_{a} \ell} \equiv \int_{0}^{\ell} d \ell^{\prime} \Sigma_{a}\left(\vec{r}-\ell^{\prime} \vec{\Omega}\right)$
It will be seen later that the usual definition of the optical path uses the total cross section. However, this amounts to the absorption cross section in this case. Just as in vacuum, only sources placed on the $\vec{\Omega}$-axis before $\vec{r}$ contribute to the angular flux in the same direction (owing to the absence of scattering). Case et al. (1953) modifies

[^145]this expression to introduce a volume integral that is more conventional to integrate. An angular Dirac function defined by:
$$
\forall \vec{\Omega}, \quad \int_{4 \pi} \delta_{2}\left(\vec{\Omega}, \vec{\Omega}^{\prime}\right) f\left(\vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}=f(\vec{\Omega})
$$
is introduced. It can also be expressed in terms of the usual Dirac distribution:
$$
\delta_{2}\left(\vec{\Omega}, \vec{\Omega}^{\prime}\right)=\frac{1}{2 \pi} \delta\left(\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)-1\right)
$$

The introduction of this angular Dirac function in the solution of the flux brings about an integration over the whole angular space:

$$
\Phi(\vec{r}, \vec{\Omega})=\int_{4 \pi} d \vec{\Omega}^{\prime} \delta_{2}(\vec{\Omega}, \vec{\Omega}) \int_{0}^{\infty} e^{-\overline{\Sigma_{a} \ell}\left(\vec{r}, \vec{\Omega}^{\prime}\right)} S\left(\vec{r}-\ell \vec{\Omega}^{\prime}, \vec{\Omega}^{\prime}\right) d \ell
$$

where the optical path is defined, with respect to the direction $\vec{\Omega}^{\prime}$, by:

$$
\overline{\Sigma_{a} \ell}\left(\vec{r}, \vec{\Omega}^{\prime}\right)=\int_{0}^{\ell} d \ell^{\prime} \Sigma_{a}\left(\vec{r}-\ell^{\prime} \vec{\Omega}^{\prime}\right)
$$

If the vector $\vec{\ell}=\ell \vec{\Omega}^{\prime}$, having volume element $\overrightarrow{d \ell}=\ell^{2} d R d \Omega^{\prime}$, is introduced, the solution for the flux can be modified so that the term for the attenuation of a point source within an absorbing medium is obtained:

Flux in a purely absorbing medium by integrating over space:

$$
\begin{equation*}
\Phi(\vec{r}, \vec{\Omega})=\int_{0}^{\infty} \delta_{2}\left(\vec{\Omega}, \frac{\vec{\ell}}{\ell}\right) e^{-\overline{\Sigma_{a} \ell}(\vec{r}, \vec{\ell})} S\left(\vec{r}-\vec{\ell}, \frac{\vec{\ell}}{\ell}\right) \frac{\overrightarrow{d \ell}}{\ell^{2}} \tag{8.15}
\end{equation*}
$$

where $\overline{\Sigma_{a} \ell}(\vec{r}, \vec{\ell})=\int_{0}^{\ell} d \ell^{\prime} \Sigma_{a}\left(\vec{r}-\vec{\ell}^{\prime}\right)$. Through this, it can be seen again that the flux in vacuum from an isotropic source placed at the origin is given by:

Flux of a point source in vacuum: $\quad \Phi(\vec{r}, \vec{\Omega})=\frac{S(\vec{r}=0, \vec{\Omega})}{r^{2}} \delta\left(\frac{\vec{r}}{r} \cdot \vec{\Omega}-1\right)$

$$
\begin{equation*}
=\frac{1}{4 \pi} \frac{S(\vec{r}=0)}{r^{2}} \delta\left(\frac{\vec{r}}{r} \cdot \vec{\Omega}-1\right) \tag{8.16}
\end{equation*}
$$

which represents the fact that neutrons are spread homogeneously over a sphere of radius $r$, and move away radially from the center. If the general case of a source $S_{0}(\vec{r}, \vec{\Omega})=S_{0} \delta_{2}\left(\vec{\Omega}, \vec{\Omega}_{0}\right) \delta\left(\vec{r}-\vec{r}_{0}\right)$ emitting solely in the $\vec{\Omega}_{0}$ direction and placed
at a point $\vec{r}_{0}$ of the absorbing medium is considered, the solution for the flux rewrites as:

$$
\Phi(\vec{r}, \vec{\Omega})=S_{0} \underbrace{\delta_{2}\left(\vec{\Omega}, \vec{\Omega}_{0}\right) \delta_{2}\left(\frac{\vec{r}-\vec{r}_{0}}{\left|\vec{r}-\vec{r}_{0}\right|}, \vec{\Omega}\right) e^{-\int_{0}^{\mid \vec{r}-\vec{r}_{0}} \mid} \Sigma_{a}\left(\vec{r}-\ell \mid \overrightarrow{r-\vec{r}_{0}}\right) d \ell}_{G\left(\vec{r}-\vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)}
$$

which shows that only neutrons emitted along the vector $\vec{r}-\vec{r}_{0}$ can reach the point $\vec{r}$, and that these contribute to the flux in the $\vec{\Omega}$ direction only when $\vec{\Omega}=\vec{\Omega}_{0}=\left(\vec{r}-\vec{r}_{0}\right) /|\vec{r}-\vec{r}|$. The term $G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)$ is similar to a Green's function [for Green's functions, the author recommends in particular (DeSanto 1992; Jerri 1999, p165; Kanwal 1971, p72 and Planchard 1995, p38 within the context of Diffusion)] which corresponds to the flux due to a unit source placed at $\vec{r}_{0}$. It is symmetric to the extent that the response in $(\vec{r}, \vec{\Omega})$, for a unit source placed at $\vec{r}_{0}$ in the $\vec{\Omega}_{0}$ direction, is the same as the response in $\left(\vec{r}_{0}-\vec{\Omega}_{0}\right)$, for a unit source placed at $\vec{r}$ in the $-\vec{\Omega}$ direction. It should be noted, mathematically, that the properties of Green's functions give:

Reciprocity theorem: $\quad G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)=G\left(\vec{r}_{0}, \vec{r},-\vec{\Omega}_{0},-\vec{\Omega}\right)$
This property, known as the reciprocity theorem, is true only for the monoenergetic transport equation, since a neutron emitted at thermal energies will not become a fast neutron at another point in the reactor, whereas the opposite is possible. The general solution for a source field will then be given by:

$$
\Phi(\vec{r}, \vec{\Omega})=\int_{0}^{\infty} d^{3} r_{0} \int_{4 \pi} d \vec{\Omega}_{0} G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right) S\left(\vec{r}_{0}, \vec{\Omega}_{0}\right)
$$

If the scattering source term now needs to be taken into account, the source term in Eq. 8.13 can be modified to give:

$$
S^{\prime}(\vec{r}, \vec{\Omega})=\int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{s}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)+S(\vec{r}, \vec{\Omega})
$$

The energy variable $E$ can be added to obtain the same equation in energy. This leads to the integral form of the equation, which contains the flux in the slowingdown term and which will be studied further later on. The complementary theorem allows for the study of the solution within a precise area: it is used in the domaindecomposition approach for particle transport, where the goal is to increase the meshing a posteriori in an area of interest. Considering a heterogeneous non-multiplicative medium surrounded by a surface $S$ and where internal and/or external sources create a flux $\Phi(\vec{r}, E, \vec{\Omega})$, the problem is mathematically equivalent
to eliminating the external sources while retaining the internal ones and adding to the surface $S$ a complementary source of intensity $-\Phi(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \cdot \vec{n}$, where $\vec{n}$ is the outside normal to $S$. Contrary to the reciprocity theorem, the complementary theorem is valid in a spectral approach to energy. It consists of replacing a source by the current it causes at the interface of interest, and is based on the linearity of the transport equation with respect to external sources. It should be cautioned here that this result is of course no longer valid if the source is coupled to the flux, i.e., in a multiplicative medium.

### 8.2.2.4 Adjoint Transport Theory

(Ferziger and Zweifel 1966, p214)

### 8.2.2.4.1 The Adjoint Integro-Differential Equation

To simplify notation, it is common in perturbation theory ${ }^{12,13}$ to define the Dirac operator $<>$ of integration over independent variables, i.e., a triple integration over space, energy and angle. Hence:

Scalar product in perturbation:

$$
\begin{equation*}
<f, g>\equiv \int_{r} \int_{E} \int_{\vec{\Omega}} f(\vec{r}, E, \vec{\Omega}) g(\vec{r}, E, \vec{\Omega}) d r d E d \vec{\Omega} \tag{8.18}
\end{equation*}
$$

The adjoint flux $\Phi^{*}$, through the very definition of the adjoint operator, satisfies the equation:

$$
<\Phi^{*}, H \Phi>\equiv<H^{*} \Phi^{*}, \Phi>
$$

where $H^{*}$ is the adjoint operator. Using only this definition, there exists an infinite number of solutions $\Phi^{*}$, since $H$ is mathematically real leading to $H^{*}=H^{T}$, and $\left.\langle\Psi, H \Phi\rangle=<H^{T} \Psi, \Phi\right\rangle$, independent of the form of $\Phi$ or $\Psi$. It is the choice of boundary conditions on the domain of interest that will restrict $\Phi^{*}$. Therefore, there are as many different adjoint fluxes as there are adjoint sources and boundary conditions. The adjoint steady-state equation of the adjoint angular flux $\Phi^{*}(\vec{r}, E,-\vec{\Omega})$ is written by considering that the neutrons are emitted by the adjoint

[^146]source-in a way considering that they are covering the inverse path of the original path while travelling back in time:
\[

$$
\begin{aligned}
& -\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}^{*}} \Phi^{*}(\vec{r}, E,-\vec{\Omega})+\Sigma_{t}(\vec{r}, E) \Phi^{*}(\vec{r}, E,-\vec{\Omega}) \\
& \quad-\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime},-\vec{\Omega}^{\prime}\right)=S^{*}\left(\vec{r}, E^{\prime},-\vec{\Omega}\right)
\end{aligned}
$$
\]

Attention is drawn to the fact that the integration variables of the slowing-down operator are swapped around, by comparison with the original equation, as well as the change in sign of the angular direction within the flux. This is because the matrix of the adjoint operator is the conjugate transpose of the matrix. If the matrix elements are real, the adjoint matrix is the matrix transposed (Glasstone and Edlund 1972, p374). This equation is rewritten by replacing $\vec{\Omega}^{\prime}$ by $-\vec{\Omega}^{\prime}$, and $\vec{\Omega}$ by $-\vec{\Omega}$ (Criticality control of fissile materials 1968, p65) and $\overrightarrow{\text { grad }^{*}}=-\overrightarrow{\text { grad }}$ (Duderstadt and Martin 1979, p371), respecting some conditions that will be detailed later:

Integro-differential equation of the adjoint flux:

$$
\begin{align*}
& -\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi^{*}(\vec{r}, E, \vec{\Omega})+\Sigma_{t}(\vec{r}, E) \Phi^{*}(\vec{r}, E, \vec{\Omega}) \\
& -\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)=S^{*}(\vec{r}, E, \vec{\Omega}) \tag{8.19}
\end{align*}
$$

This equation is rigorously identical in form to the direct equation, except that the slowing-down operator is written with the transposed matrix and the sign change of the leakage operator. Creating the adjoint of the transport equation requires a detailed explanation. The absorption term $\Sigma_{t}(\vec{r}, E) \Phi(\vec{r}, E, \vec{\Omega})$, being self-adjoint, its equivalent in the adjoint equation is hence $\Sigma_{t}(\vec{r}, E) \Phi^{*}(\vec{r}, E, \vec{\Omega})$. It is easily seen that the adjoint of the scattering operator $\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime}, \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)$ is obtained by substituting the prime indices of the energy and direction variables, while noticing that:

$$
\begin{aligned}
& \int_{r} d^{3} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \Phi^{*}(\vec{r}, E, \vec{\Omega}) \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}^{\prime}, \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) \\
& =\int_{r} d^{3} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \Phi(\vec{r}, E, \vec{\Omega}) \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} . \vec{\Omega}^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

Finding the adjoint of the leakage operator $\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, E, \vec{\Omega})$ is trickier. Noticing that:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E, \vec{\Omega})=\operatorname{div}(\vec{\Omega} \cdot \Phi(\vec{r}, E, \vec{\Omega}))-\Phi(\vec{r}, E, \vec{\Omega}) \underbrace{\operatorname{div}(\vec{\Omega})}_{0}
$$

since $\vec{\Omega}$ is a direction constant in the equation, and that similarly:

$$
\begin{aligned}
\Phi^{*}(\vec{r}, E, \vec{\Omega}) \cdot \operatorname{div}(\vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega}))= & \operatorname{div}\left(\vec{\Omega} \cdot \Phi(\vec{r}, E, \vec{\Omega}) \Phi^{*}(\vec{r}, E, \vec{\Omega})\right) \\
& -\Phi(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}(\vec{r}, E, \vec{\Omega})
\end{aligned}
$$

the scalar product can be rewritten as:

$$
\begin{aligned}
& \int_{r} d^{3} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega}) \\
& \quad=\int_{r} d^{3} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \operatorname{div}\left(\Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega})\right) \\
& \quad-\int_{r} d^{3} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \Phi(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi^{*}(\vec{r}, E, \vec{\Omega})
\end{aligned}
$$

The second term on the right-hand side corresponds to the operator $-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}}$ $\Phi^{*}(\vec{r}, E, \vec{\Omega})$ of the adjoint equation while the first term can be replaced by an integral over the surface of the reactor, thanks to Ostrogradsky (divergence) theorem:

$$
\begin{aligned}
& \int_{r} d^{3} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \operatorname{div}\left(\Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega})\right) \\
& \quad=\int_{r_{S}} d^{2} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \vec{n} \cdot\left(\Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega})\right)
\end{aligned}
$$

This surface integral can be broken down into two integrals, one for the incoming directions $\vec{\Omega} . \vec{n}<0$, where $\vec{n}$ is the outside normal to the surface reactor, and another for the outgoing directions $\vec{\Omega} . \vec{n}>0$ :

$$
\begin{aligned}
& \int_{r_{S}} d^{2} r \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E \vec{n} \cdot\left(\Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega})\right) \\
& =\int_{r_{S}} d^{2} r \int_{\vec{\Omega} \cdot \vec{n}<0} d \vec{\Omega} \int_{0}^{\infty} d E \vec{n} \cdot\left(\Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega})\right) \\
& \quad+\int_{r_{S}} d^{2} r \int_{\vec{\Omega} \cdot \vec{n}>0} d \vec{\Omega} \int_{0}^{\infty} d E \vec{n} \cdot\left(\Phi^{*}(\vec{r}, E, \vec{\Omega}) \vec{\Omega} \Phi(\vec{r}, E, \vec{\Omega})\right)
\end{aligned}
$$

For the incoming directions, the angular flux will be zero if the surface is convex, and if the reactor is surrounded by vacuum or a completely-absorbing medium
(black body). For outgoing directions, it can be imposed that it is the adjoint angular flux that should be zero, by imposing that as boundary condition for the problem. This leads to the following boundary conditions:

$$
\left\{\begin{array}{ccc}
\Phi\left(\vec{r}_{S}, E, \vec{\Omega}\right)=0 & \text { for } & \vec{\Omega} \cdot \vec{n}<0 \\
\Phi^{*}\left(\vec{r}_{S}, E, \vec{\Omega}\right)=0 & \text { for } & \vec{\Omega} \cdot \vec{n}>0
\end{array}\right.
$$

It should be noted that if a too restrictive condition is applied, such as:

$$
\Phi\left(\vec{r}_{S}, E, \vec{\Omega}\right)=0 \quad \forall \vec{\Omega} \quad \text { or } \quad \Phi^{*}\left(\vec{r}_{S}, E, \vec{\Omega}\right)=0 \quad \forall \vec{\Omega}
$$

this means that the integrated flux (or the adjoint integrated flux) is zero at the interface, which is consistent in a homogeneous medium only with a subcritical reactor, hence not in steady-state by definition. Regarding the source term, an isotropic fission term is written as:

$$
\chi(E) \int_{0}^{\infty} d E^{\prime} v \Sigma_{f}\left(\vec{r}, E^{\prime}\right) \int_{4 \pi} d \vec{\Omega}^{\prime} \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
$$

the adjoint term of which, using a reasoning analogous to that used for the scattering term, is given by:

$$
v \Sigma_{f}(\vec{r}, E) \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \chi\left(E^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
$$

Finally, the adjoint equation of the critical equation with fission sources, assuming that the incoming flux and the adjoint outgoing flux are zero, is written as:

$$
\begin{aligned}
& -\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi^{*}(\vec{r}, E, \vec{\Omega})+\Sigma_{t}(\vec{r}, E) \Phi^{*}(\vec{r}, E, \vec{\Omega}) \\
& -\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \overrightarrow{\Omega^{\prime}} \Sigma_{S}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) \\
& \quad=\nu \Sigma_{f}(\vec{r}, E) \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \chi\left(E^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

If the incoming flux is non-zero, which is the case at the active core-reflector interface, the adjoint term $-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}(\vec{r}, E, \vec{\Omega})$ is not so rigorous anymorewhich is an easily overlooked fact.

In multi-group, the original operator is written:

$$
\int_{4 \pi} d \vec{\Omega}^{\prime} \sum_{g^{\prime}} \Sigma_{g^{\prime} \rightarrow g}\left(\vec{\Omega}^{\prime} . \vec{\Omega}\right) \Phi_{g^{\prime}}\left(\vec{r}, \vec{\Omega}^{\prime}\right)
$$

while the adjoint operator is $\int_{4 \pi} d \vec{\Omega}^{\prime} \sum_{g^{\prime}} \Sigma_{g \rightarrow g^{\prime}}\left(\vec{\Omega}^{\prime} . \vec{\Omega}\right) \Phi_{g^{\prime}}^{*}\left(\vec{r}, \vec{\Omega}^{\prime}\right)$.

It will be noted that the adjoint flux is dimensionless if the adjoint source has the same dimensions as a cross section, but that it could be otherwise for another type of adjoint source-which can create some confusion. Numerous texts use the concept of adjoint flux without clearly explaining the defining conditions for this flux (giving the impression that it were unique, similarly to the original flux), which again is a cause for widespread confusion. The adjoint flux acts as a weight function, which represents the contribution of a neutron to a given response (for example, a detector, in which case the adjoint source will be the surface area of the detector). The adjoint flux associated with a null condition on the edge for a homogeneous medium is called the fundamental adjoint flux. It is known, just like the original flux, only up to a multiplicative constant. Hence, the adjoint flux depends on the adjoint source, and there are as many adjoint flux profiles as there are possible adjoint sources (and boundary conditions imposed on the adjoint flux). Therefore, it is preferable to never mention adjoint fluxes without specifying the nature of the corresponding adjoint source and the boundary condition, otherwise the problem would be (mathematically) ill-posed. Attention will be drawn to the prime indices on the energy variable $E^{\prime}$ of the scattering source term, which are "inversed" with respect to the original flux equation (which amounts to taking the transpose of the matrix associated with the slowing-down operator). The integration over angle of the adjoint equation leads to:

$$
\begin{aligned}
& -\int_{4 \pi} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}(\vec{r}, E, \vec{\Omega}) d \vec{\Omega}+\int_{4 \pi} \Sigma_{t}(\vec{r}, E) \Phi^{*}(\vec{r}, E, \vec{\Omega}) d \vec{\Omega} \\
& -\int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega} . . \vec{\Omega}^{\prime}\right) \Phi^{*}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)=\int_{4 \pi} S^{*}(\vec{r}, E, \vec{\Omega}) d \vec{\Omega}
\end{aligned}
$$

Compelling applications of the adjoint flux in perturbation theory will be discussed later.

### 8.2.2.4.2 The Adjoint Equation for the Computation of Neutron Multiplication

A possible use of adjoint theory is the problem of the contribution to leakage by a neutron emitted at $\vec{r}$ with energy $E$. An adjoint equation can be set up by considering the number $p(\vec{r}, E, \vec{\Omega})$ of neutrons lost by leakage from the system, induced by the previously mentioned neutron emitted in the $\vec{\Omega}$ direction (Careful! This is not the leakage probability; indeed, this number of neutrons can be higher than 1.). The differential equation for this variable is:

$$
\begin{aligned}
& p(\vec{r}, E, \vec{\Omega})=p(\vec{r}+\ell \vec{\Omega}, E, \vec{\Omega}) \times \underbrace{e^{-\overline{\Sigma_{\ell} \ell}}}_{\begin{array}{l}
\text { probability of non-interaction } \\
\text { in the path } \ell
\end{array}} \\
& +\underbrace{}_{\underbrace{\ell^{\prime}=0} e^{\ell^{\prime}=\ell} e^{-\overline{\Sigma_{t}\left(\ell-\ell^{\prime}\right)}} d \ell^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} c \Sigma_{t}\left(\vec{r}+\ell^{\prime} \vec{\Omega}, E \rightarrow E^{\prime}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right) p\left(\vec{r}+\ell^{\prime} \vec{\Omega}, E^{\prime}, \vec{\Omega}^{\prime}\right)}
\end{aligned}
$$

neutrons coming from the medium in the correct direction and created by collision by the initial neutron of energy E along the path $\ell$ and arriving in $\vec{r}+\ell \vec{\Omega}$ while leaving from $\vec{r}+\ell^{\prime} \vec{\Omega}$

Parameter $c$ is the number of secondary neutrons emitted by collision (Silvennoinen 1976, p37). Since $e^{\overline{-\Sigma_{t} \ell}}=1-\Sigma_{t} \ell+O\left(\ell^{2}\right)$, rearranging the previous equation and writing it to first order gives:

$$
\begin{aligned}
& \frac{p(\vec{r}, E, \vec{\Omega})-p(\vec{r}+\ell \vec{\Omega}, E, \vec{\Omega})}{\ell}+\Sigma_{t} p(\vec{r}+\ell \vec{\Omega}, E, \vec{\Omega}) \\
& \quad=\int_{4 \pi} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} c \Sigma_{t}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right) p\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

Considering the limiting case of $\ell$ tending to zero, the adjoint integro-differential equation for the number of neutrons lost by leakage is obtained:

Equation for the number of neutrons leaked: $\quad-\frac{\partial p(\vec{r}, E, \vec{\Omega})}{\partial \ell}+\Sigma_{t} p(\vec{r}, E, \vec{\Omega})=$

$$
\begin{equation*}
-\vec{\Omega} . \overrightarrow{g r a d} p(\vec{r}, E, \vec{\Omega})+\Sigma_{t} p(\vec{r}, E, \vec{\Omega})=\int_{4 \pi} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} c \Sigma_{t}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right) p\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) \tag{8.20}
\end{equation*}
$$

If the medium is geometrically convex, a $4 \pi$-source point $\vec{r}_{S}$ on its surface $S$ will have its number of neutrons lost by leakage $p\left(\vec{r}_{S}, E, \vec{\Omega}\right)=1$ for $\vec{\Omega} . \vec{n}>0$, where $\vec{n}$ is the outside normal to the volume (outgoing directions), since a neutron emitted in this direction will not be able to re-enter the system because of its convexity. Comparing (8.20) to the adjoint equation (8.19), it can be seen that they are identical, with $p(\vec{r}, E, \vec{\Omega})=\Phi^{*}(\vec{r}, E,-\vec{\Omega})$ and $S^{*}(\vec{r}, E, \vec{\Omega})=\nu \Sigma_{f} \Phi^{*}(\vec{r}, E, \vec{\Omega})$, i.e., taking into account only fission sources. The number of neutrons lost by leakage can hence be calculated by solving the adjoint integro-differential equation, with the fission source as the adjoint source, and with the boundary condition $\Phi^{*}(\vec{r}, E, \vec{\Omega})=1$ for incoming directions $\vec{\Omega} . \vec{n}<0$.

Solving the problem in multi-group will lead to the system of equations:

$$
-\vec{\Omega} \cdot \overrightarrow{g r a d} p_{g}(\vec{r}, \vec{\Omega})+\Sigma_{t, g} p_{g}(\vec{r}, \vec{\Omega})=\int_{4 \pi} d \vec{\Omega}^{\prime} \sum_{g^{\prime}=1}^{G} c_{g} \Sigma_{t, g}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) p_{g}\left(\vec{r}, \vec{\Omega}^{\prime}\right)
$$

with $p_{g}\left(\vec{r}_{S}, \vec{\Omega}\right)=\delta_{g, h} \quad$ for $\vec{\Omega} . \vec{n}>0$ as boundary condition, which leads to the contribution to leakage from a source of 1 neutron per second placed at $\vec{r}$ in the energy group $h$. To obtain the contribution from all the groups of a multi-energetic source over the set of $G$ groups, (unfortunately) $G$ adjoint calculations have to be carried out, which decreases the appeal of the method with respect to a direct approach by modifying the boundary condition.

### 8.2.2.4.3 Neutron Importance

(Stacey 2001, p485; Reuss 2003, p370)
It is often interesting to look at the neutron importance, i.e., the contribution of a neutron emitted at $\vec{r}$, with energy $E$ to the multiplication of a system. It is thanks to Eugene Wigner that the physical meaning of this particular adjoint flux was identified as early as 1945. It can easily be understood that a neutron emitted at the surface of a convex system towards outgoing directions will not be able to contribute to the system multiplication. The boundary condition of the importance $I(\vec{r}, E, \vec{\Omega})$ therefore concerns the outgoing directions:

$$
\forall E, I\left(\vec{r}_{S}, E, \vec{\Omega}\right)=0 \quad \text { pour } \vec{\Omega} . \vec{n}>0
$$

The neutron importance will therefore be stronger in the reactor center than on the periphery, and stronger at thermal energies-where the fission probability is very high-than at a capture resonance energy, where the neutron has every chance of being captured. Following the same reasoning as in the previous paragraph, the neutron importance will satisfy the adjoint equation with the (transposed) fission source as adjoint source (Fig. 8.8):

Neutron importance equation: $\quad-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} I(\vec{r}, E, \vec{\Omega})+\Sigma_{t} I(\vec{r}, E, \vec{\Omega})=$

$$
\begin{equation*}
\int_{4 \pi} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} c \Sigma_{t}\left(\vec{r}, E \rightarrow E^{\prime}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right) I\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) \tag{8.21}
\end{equation*}
$$

In this equation, the expression $c \Sigma_{t}\left(E \rightarrow E^{\prime}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right) \equiv \chi\left(E^{\prime}\right) \nu \Sigma_{f}(E)+$ $\Sigma_{s}\left(E \rightarrow E^{\prime}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right)$ where parameter $c$ is the number of secondary neutrons, is corresponding in the adjoint equation of the expression $c \Sigma_{t}\left(E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \equiv$ $\chi(E) \nu \Sigma_{f}\left(E^{\prime}\right)+\Sigma_{s}\left(E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right)$ included in the direct equation.

Fig. 8.8 Variation of the importance in the energy neighbourhood of a resonance: a scattering resonance does not modify the importance


Following expressions should be used as boundary condition on all incoming directions and all energies:

$$
\forall E, I\left(\vec{r}_{S}, E, \vec{\Omega}\right)=0 \quad \text { for } \vec{\Omega} . \vec{n}<0
$$

It is interesting to note that, in all likelihood, $I\left(\vec{r}_{S}, E, \vec{\Omega}\right)>0$ for $\vec{\Omega} . \vec{n}>0$, which, upon integrating over $4 \pi$ steradians, gives a non-zero integrated importance $I\left(\vec{r}_{S}, E\right)$ on the reactor surface. An adjoint flux calculation with a zero adjoint flux on the boundary therefore does not yield the importance, contrary to widespread belief leading to incorrect modelization in some codes. It is essential to understand that the importance has meaning only for a critical reactor. Physically, the importance $I(\vec{r}, E, \vec{\Omega})$ is proportional to the total number of neutrons that are produced by introducing a neutron at the point $\vec{r}$, with energy $E$, and in the direction $\vec{\Omega}$. In a supercritical reactor, this value tends to infinity. In a subcritical reactor, it tends to zero. In a critical reactor where a source is inserted, the problem cannot have a steady-state solution, owing to the strict positivity of the importance.

### 8.2.2.4.4 Perturbation Theory Approach to the Subcritical Flux with Source

In a very slightly subcritical reactor, if a source of 1 neutron per second is located at the same point of the phase space, the obtained equilibrium distribution will be such that the total number of neutrons will be proportional to the calculated importance for the nearly-critical reactor. If the reactor is 'too' subcritical, the permanent adjoint flux, even if calculated with the boundary condition of the importance, will not be representative of the latter anymore. The adjoint flux becomes a purely mathematical concept, which does not have physical meaning anymore, and the


Fig. 8.9 Jacques Planchard (1933-2009) is one of the greatest authorities on numerical methods as applied to nuclear reactors. He joined EDF R\&D in 1956 following a degree in mathematics. He is credited with much of the important work on direct and inverse perturbation methods, eigenvalue calculations or non-coupled source calculations. He is the author of a very thorough book on these topics in 1995 "Méthodes mathématiques en neutronique" [Mathematical methods in neutronics], book which contains original derivations, particularly on convergence problems, which is a topic that has received little attention in literature. This is why he is one of the pillars of "mathematical" neutronics in France. Anecdotally, he would carry on going to work for free, years after his retirement, so much his work was dear to him. (Picture of Planchard at the summer school of Numerical Analysis in Bréau sans Nappe in 1970, courtesy of Guy Blanchon)
problem, even if it converges, is ill-posed. This is not a purely academic matter, since during the transition phase of subcritical to critical for a reactor, the flux depends on the location and intensity of external sources, while the reactivity depends solely on the state of the reactor, and is hence independent of the sources. ${ }^{14}$ With an external source $S(\vec{r}, E)$, the only steady-state problem is written (Fig. 8.9):

$$
\begin{align*}
& \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{\varepsilon}(\vec{r}, E, \vec{\Omega})+\Sigma_{t} \Phi_{\varepsilon}(\vec{r}, E, \vec{\Omega}) \\
& =\int_{4 \pi} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} c \Sigma_{t}\left(E^{\prime} \rightarrow E, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}\right) \Phi_{\varepsilon}\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) d \vec{\Omega} \\
& \quad-\varepsilon \nu \Sigma_{f}(E,) \Phi_{\varepsilon}(\vec{r}, E)+S(\vec{r}, E) \tag{8.22}
\end{align*}
$$

where $\varepsilon \in[0,1]$ is the anti-reactivity of the reactor. If $\varepsilon$ tends to zero, the flux $\Phi_{\varepsilon}(\vec{r}, E)$, where the index explicitly shows that it depends on $\varepsilon$, tends to infinity, unless the source itself tends to zero. If considered to first order, the source tends to zero, i.e., $S(\vec{r}, E)=\varepsilon S_{0}(\vec{r}, E)$, then the flux tends to the solution of the critical

[^147]calculation without external sources. Planchard suggests ${ }^{15}$ developing the subcritical mono-energetic flux in the form of a diverging series when $\varepsilon \rightarrow 0$ :
$$
\Phi_{\varepsilon}(\vec{r})=\alpha_{0} \Phi(\vec{r})+\varepsilon \Psi_{1}(\vec{r})+\varepsilon^{2} \Psi_{2}(\vec{r})+\ldots
$$
where $\Phi(\vec{r})$ is the flux from the critical calculation. Writing Eq. 8.22 to one energy group, in operator form, leads to:
$$
[K-(1-\varepsilon) P]\left[\Phi_{\varepsilon}(\vec{r})\right]=S(\vec{r})
$$

By replacing the flux and source in this equation by their Taylor expansion in $\varepsilon$, and then identifying the coefficients on either side of the polynomial obtained, we find:

$$
\left\{\begin{array}{l}
{[K-P]\left[\Psi_{1}(\vec{r})\right]=-\alpha_{0} P \Phi(\vec{r})+S_{0}(\vec{r})} \\
{[K-P]\left[\Psi_{2}(\vec{r})\right]=-P \Psi_{1}(\vec{r})} \\
\vdots \\
{[K-P]\left[\Psi_{n+1}(\vec{r})\right]=-P \Psi_{n}(\vec{r})}
\end{array}\right.
$$

Since the operator matrix $[K-P]$ is singular for the critical problem, we will use this property by multiplying the first equation of the system by an adjoint flux (for example, the importance), verifying the adjoint equation with a fission source but no independent sources. The orthogonality property with respect to the scalar product of the adjoint flux allows us to find:

$$
\alpha_{0}=\frac{\left\langle S_{0}, \Phi^{*}\right\rangle}{\left\langle P \Phi, \Phi^{*}\right\rangle}
$$

Starting with $\alpha_{0}$ which is already known, $\Psi_{1}(\vec{r})$ can be uniquely written in the form $\Psi_{1}(\vec{r})=\Psi_{1,0}(\vec{r})+\alpha_{1} \Phi(\vec{r})$ where $\Psi_{1,0}(\vec{r})$ is a unique solution in the space orthogonal to $\Phi(\vec{r})$. We can then compute:

$$
\alpha_{1}=\frac{\left\langle P \Psi_{1,0}, \Phi^{*}\right\rangle}{\left\langle P \Phi, \Phi^{*}\right\rangle}
$$

and so on from one to the other using relations such as $\Psi_{2}(\vec{r})=\Psi_{2,0}(\vec{r})+\alpha_{2} \Phi(\vec{r})$. It can be seen how using the orthogonality condition allows for calculating the perturbed flux $\Phi_{\varepsilon}(\vec{r})$ in the form of a truncated Taylor series in $\varepsilon$. If the perturbation is important, the terms orthogonal to $\Phi(\vec{r})$ have more weight, representing a gain in

[^148]amplitude of the non-fundamental harmonics. We note here that Chap. 17 will address the problem of a sub-critical approach again.

### 8.2.2.5 The Critical Reactor Eigenvalue Problem

(Planchard 1985)
To determine the criticality of a reactor, an eigenvalue problem is used once more, to find the largest eigenvalue of the effective multiplication factor $k_{\text {eff }}$, such that the steady-state integro-differential equation is satisfied:
$\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})=$

$$
\begin{equation*}
\int_{0}^{\infty} d E \int_{0}^{\infty} d E^{\prime} \int_{\vec{\Omega}^{\prime}} d \overrightarrow{\Omega^{\prime}} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \overrightarrow{\Omega^{\prime}}\right)+\frac{\nu \Sigma_{f}(\vec{r}) \iint_{\overrightarrow{\Omega^{\prime}}} d \overrightarrow{\Omega^{\prime}} \Phi\left(\vec{r}, \overrightarrow{\Omega^{\prime}}\right)}{k_{e f f}} \tag{8.23}
\end{equation*}
$$

Taking into account the energy variable, the fission spectrum $\chi(E)$ appears and is independent of the energy of the incident neutron:

$$
\begin{aligned}
\vec{\Omega} . \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega}, E)+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega}, E)= & \int_{0}^{\infty} d E^{\prime} \int_{\vec{\Omega}^{\prime}} d \overrightarrow{\Omega^{\prime}} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \overrightarrow{\Omega^{\prime}}\right) \\
& +\chi(E) \int_{E^{\prime}} d E^{\prime} \int_{\vec{\Omega}^{\prime}} d \overrightarrow{\Omega^{\prime}} \frac{\nu\left(E^{\prime}\right) \Sigma_{f}\left(\vec{r}, E^{\prime}\right) \Phi\left(\vec{r}, \overrightarrow{\Omega^{\prime}}, E^{\prime}\right)}{k_{e f f}}
\end{aligned}
$$

The only way a steady-state solution exists is if $k_{\text {eff }}=1$. Equation 8.23 can be written in a condensed form by using the operators of Eq. 8.10, which allows us to compute the flux using the general formula:

$$
\Phi=H^{-1}\left(\frac{\chi}{k_{e f f}} \nu \Sigma_{f} \Phi\right) .
$$

The effective multiplication factor can then be expressed in the general form:

$$
k_{e f f}=\frac{\int_{E^{\prime}} d E^{\prime} \int_{\overrightarrow{\Omega^{\prime}}} d \overrightarrow{\Omega^{\prime}} \nu\left(E^{\prime}\right) \Sigma_{f}\left(\vec{r}, E^{\prime}\right) H^{-1}\left(\chi \nu \Sigma_{f} \Phi\right)}{\int_{E^{\prime}} d E^{\prime} \int_{\vec{\Omega}^{\prime}} d \overrightarrow{\Omega^{\prime}} \nu\left(E^{\prime}\right) \Sigma_{f}\left(\vec{r}, E^{\prime}\right) H^{-1}\left(\frac{\chi}{k_{e f f}} \Sigma_{f} \Phi\right)} .
$$

A conventional way of calculating the eigenvalue is to use the power iteration method which consists of iterating over the fission term, starting with the initial coefficient set $\left(\Phi^{0}, k_{\text {eff }}^{0}\right)$. Assuming the following:

$$
\nu \Sigma_{f} \Phi^{n}=\frac{1}{k_{e f f}^{n-1}} \int_{E^{\prime}} d E^{\prime} \int_{\Omega_{\Omega^{\prime}}} d{\overrightarrow{\Omega^{\prime}}}^{\prime} \nu\left(E^{\prime}\right) \Sigma_{f}\left(\vec{r}, E^{\prime}\right) H^{-1}\left(\chi \nu \Sigma_{f} \Phi^{n-1}\right)
$$

we solve iteratively the equation below:

$$
H \Phi^{n}=\frac{\chi}{k_{e f f}^{n-1}} \nu \Sigma_{f} \Phi^{n-1}
$$

The new value $k_{\text {eff }}^{n}$ is obtained by iteration by using the scalar product of functions, integrated over the reactor,

$$
<f(\vec{r}), g(\vec{r})>\equiv \int_{\text {reacteur }} f(\vec{r}) g(\vec{r}) d \vec{r}
$$

yielding,

$$
k_{e f f}^{n}=k_{e f f}^{n-1} \frac{\left\langle\nu \Sigma_{f} \Phi^{n}, w\right\rangle}{\left\langle\nu \Sigma_{f} \Phi^{n-1}, w\right\rangle}
$$

where $w(\vec{r})$ is a weight function carefully chosen to accelerate the convergence rate.

### 8.2.2.6 Uncollided Flux

### 8.2.2.6.1 Green's Functions, Uncollided Neutron Flux

(Shultis and Faw 2000, p156)
When the total cross section is used in the calculation of the optical path, it comes down to eliminating the neutrons that undergo the slightest collisionwhether it be absorption or scattering-in the calculation of the neutron population in a given direction. The terms first-flight neutrons and first-flight flux are used, or simply uncollided flux. Thanks to the linearity of the Boltzmann transport equation,
the flux solution can be reconstructed in a space containing imposed sources, using combinations of basic solutions of plane or point sources. Hence it is interesting to determine the first-flight kernels, solutions to the integro-differential equation, i.e., the Green's functions of some particular simple geometries. Recall that the Green's function $G\left(\vec{r}, \vec{r}_{0}\right)$ represents in our case the flux at $\vec{r}$ when a unit point source is placed at $\vec{r}_{0}$. For example, for a conventional diffusion operator, this function satisfies:

$$
\begin{equation*}
\text { Green's function for diffusion: }-D \Delta G\left(\vec{r}, \vec{r}_{0}\right)+\Sigma_{a} G\left(\vec{r}, \vec{r}_{0}\right)=\delta\left(\vec{r}-\vec{r}_{0}\right) \tag{8.24}
\end{equation*}
$$

The Green's function depends not only on the form of the differential equation but also on the boundary conditions (zero at infinity, or on a boundary of the domain, etc.) (Kanwal 1971, p106). For monoenergetic neutrons, $G\left(\vec{r}, \vec{r}_{0}\right)=$ $G\left(\vec{r}_{0}, \vec{r}\right)$. This can be generalized by introducing an angular variable; $G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}_{0}\right)$ is then the flux at $\vec{r}$ in the direction $\vec{\Omega}$ produced by a source at $\vec{r}_{0}$ emitting in the direction $\vec{\Omega}_{0}$. For a source spread over a volume $V$, the resulting flux will be obtained by integrating the product of the source and the Green's function over the volume, because of the linearity of the diffusion equation, leading to:

$$
\Phi(\vec{r}, \vec{\Omega})=\int_{V} \int_{\vec{\Omega}^{\prime}} \vec{d}^{\prime} G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) S\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}\right)
$$

Since the transport operator is linear as well, similarly a Green's function associated with it can be defined. This Green's function will be, of course, different from that for the diffusion equation since it is associated with the operator via Eq. 8.24. It has already been seen that the angular flux of an isotropic source is given by Eq. 8.16.

### 8.2.2.6.2 Uncollided Flux from a Point Source

In a medium with total cross section $\Sigma_{t}$, the first-flight flux induced by an isotropic source $S_{0} /(4 \pi)$ is given by:

$$
\Phi_{u n c}(\vec{r}, \vec{\Omega})=\int_{0}^{\infty} d^{3} r_{0} \int_{4 \pi} d \overrightarrow{\Omega_{0}} \quad G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \overrightarrow{\Omega_{0}}\right) S\left(\vec{r}_{0}, \overrightarrow{\Omega_{0}}\right)
$$

with: $G\left(\vec{r}, \vec{r}_{0}, \vec{\Omega}, \overrightarrow{\Omega_{0}}\right)=\delta_{2}\left(\vec{\Omega}, \overrightarrow{\Omega_{0}}\right) \delta_{2}\left(\frac{\vec{r}-\vec{r}_{0}}{\left|\vec{r}-\overrightarrow{r_{0}}\right|}, \vec{\Omega}\right) e^{-\int_{0}^{\left|\vec{r}-\vec{r}_{0}\right|} \Sigma_{t}\left(\vec{r}-\ell \frac{\vec{r}-\vec{r}_{0}}{\left|\vec{r}-\vec{r}_{0}\right|}\right) d \ell}$ and $S\left(\vec{r}_{0}, \vec{\Omega}_{0}\right)=\frac{S_{0}}{4 \pi} \delta\left(\vec{r}, \vec{r}_{0}\right)$.

Fig. 8.10 Isotropic source placed in an absorbing and scattering medium


By placing the source at the center of the reference frame, i.e., $\vec{r}_{0}=0$, the calculation is simplified (Fig. 8.10):

$$
\Phi_{\text {unc }}(\vec{r}, \vec{\Omega})=\frac{S_{0}}{4 \pi} \delta_{2}\left(\frac{\vec{r}}{r} \cdot \vec{\Omega}\right) e^{-\int_{0}^{r} \Sigma_{l}\left(\vec{r}-\ell \frac{\vec{r}}{r}\right) d \ell}
$$

It should be noted that the uncollided flux should not be confused with the real flux. The crucial difference stems from the fact that the real flux comprises the contribution of neutrons scattered from any point of the scattering medium. If the uncollided flux is integrated over all directions, it is found for a medium of constant total cross section:

First-flight flux for a point source: $\quad \Phi_{\text {unc }}^{\text {ponctual }}(r)=$

$$
\begin{equation*}
\int_{4 \pi} d \vec{\Omega} \frac{S_{0}}{4 \pi} \delta_{2}\left(\frac{\vec{r}}{r}, \vec{\Omega}\right) e^{-\int_{0}^{r} \Sigma_{t}(\vec{r}-\ell \vec{r}) d \ell}=\frac{S_{0}}{4 \pi r^{2}} e^{-\Sigma_{t} r} \tag{8.25}
\end{equation*}
$$

This intuitive result spreads the neutron flux in an isotropic way over a surface of $4 \pi r^{2}$ by taking into account an attenuation coefficient, which is actually the total macroscopic cross section. It should be pointed out that this flux tends to infinity when $r \rightarrow 0$ while the uncollided neutron current stays finite. This suggests that the flux, in transport theory, which is composed of the first-flight flux and the contributions to the flux due to the successive collisions, will itself tend to infinity in the neighborhood of the source. This remark is to draw the reader's attention on the fact that the definition of the flux remains a volumetric concept, which loses meaning once indefinitely close to the source. The purely mathematic idealization of the point source emitting neutrons that physically occupy a volume in space should also be noted. Hence, there very well exists a limiting radius under which the notion of flux is not a physical concept anymore.

If the medium is purely absorbing (no scattering), the uncollided flux becomes the real flux by replacing the total cross section by the absorption cross section. The neutron current in any given direction $\vec{\Omega}$ is given by:

$$
\vec{J}(r, \vec{\Omega})=\frac{S_{0}}{4 \pi r^{2}} e^{-\Sigma_{t} r} \delta_{2}\left(\frac{\vec{r}}{r}, \vec{\Omega}\right) \frac{\vec{r}}{r}
$$

which represents the fact that the uncollided current is in the direction given by the vector $\vec{\Omega}=\vec{r} / r$ (and zero in all other directions).

### 8.2.2.6.3 Uncollided Flux from a Plane Source

From the mathematical construct of the point source, the uncollided flux of a plane source can be calculated by simple integration. The uncollided flux induced by an isotropic plane source is obtained by integrating the effect of a point source corresponding to an elementary ring of thickness $d r$ (Stacey 2001, p303):

$$
\Phi_{\text {unc }}^{\text {plane }}(x)=\int_{r=0}^{+\infty} \Phi_{\text {unc }}^{\text {ponctual }}(R) 2 \pi r d r
$$

By assuming that the source emits $S_{0} / 2$ neutrons per second and per unit surface in the right half-space, and since $R^{2}=r^{2}+x^{2}$, after integration over $R$, it is found that:

$$
\Phi_{\text {unc }}^{\text {plane }}(x)=\int_{r=0}^{+\infty} \Phi_{\text {unc }}^{\text {ponctual }}(R) 2 \pi r d r=\frac{S_{0}}{2} \int_{R=x}^{R=+\infty} \frac{e^{-\Sigma_{t} R}}{R} d R=\frac{S_{0}}{2} E_{1}\left(\Sigma_{t} x\right),
$$

It should be noted that an exponential function ${ }^{16}$ was used. The latter can only be computed numerically and is given by (Fig. 8.11):

$$
\begin{equation*}
\text { Exponential function: } \quad E_{n}(x) \equiv \int_{1}^{+\infty} y^{-n} e^{-y x} d y=\int_{0}^{1} \mu^{n-2} e^{-\frac{x}{\mu}} d \mu \tag{8.26}
\end{equation*}
$$

The positive uncollided current, going through a surface element placed at $x$ and parallel to the source place, is obtained by integration of the current from a point source:

[^149]

Fig. 8.11 Isotropic plane source

$$
\left\{\begin{array}{l}
J^{+}(x)=\int_{r=0}^{+\infty} \Phi_{\text {unc }}^{\text {ponctual }}(R) \underbrace{\vec{\Omega} \cdot \vec{n}}_{\cos \theta=\frac{x}{R}} 2 \pi \underbrace{r d r}_{R d R}=x \frac{S_{0}}{2} \int_{R=x}^{R=+\infty} \frac{e^{-\Sigma_{l} R}}{R^{2}} d R=\frac{S_{0}}{2} \int_{y=1}^{y=+\infty} \frac{e^{-\Sigma_{r} x y}}{y^{2}} d y=\frac{S_{0}}{2} E_{2}\left(\Sigma_{t} x\right) \\
J^{-}(x)=0
\end{array}\right.
$$

### 8.2.2.6.4 Uncollided Flux from an Isotropic Line Source

In the same way, we can compute the uncollided flux from a line source (Stacey 2001, p309):

Since $R^{2}=r^{2}+x^{2}$, we have $R d R=x d x$, and $\operatorname{since} \sin \varphi=r / R$ and $\cos \varphi=x / R$, we obtain $d \varphi=-r d x / R^{2}$. In this way, an integral over the $x$ coordinate of the line is transformed into an integral over the angle $\varphi$ between the line and segment $X M$ (Fig. 8.12).

$$
\begin{aligned}
\Phi_{\text {unc }}^{\text {line }}(x) & =\int_{x=-\infty}^{+\infty} \Phi_{\text {unc }}^{\text {ponctual }}(R) d x=2 \int_{x=0}^{+\infty} \frac{S_{0}}{4 \pi R^{2}} e^{-\Sigma_{t} R} d x \\
& =\frac{S_{0}}{2 \pi r} \int_{\varphi=0}^{\pi / 2} e^{-\frac{\Sigma_{t} r}{\sin \varphi}} d \varphi=\frac{S_{0}}{2 \pi r} K i_{1}\left(\Sigma_{t} r\right)
\end{aligned}
$$

In this, a Bickley-Nayler function of order 1 has been used, with the general form being given by (Silvennoinen 1976, p165):

Fig. 8.12 Isotropic line source


Bickley-Nayler functions:

$$
\begin{equation*}
K i_{n}(x) \equiv \int_{0}^{\frac{\pi}{2}}(\sin \varphi)^{n-1} e^{-\frac{x}{\sin \varphi}} d \varphi=\int_{0}^{\frac{\pi}{2}}(\cos \theta)^{n-1} e^{-\frac{x}{\cos \theta}} d \theta \tag{8.27}
\end{equation*}
$$

The uncollided flux can be calculated for a large number of geometries by combining the uncollided fluxes of the simple geometries that have just been detailed.

### 8.2.2.6.5 Using Homogeneous Green’s Functions

Moving along a direction $\vec{\Omega}$, the flux is continuous through an interface separating two media. Regions containing a homogeneous and isotropic medium are chosen here to tile the space. Considering the Heaviside function (step function) ${ }^{17}$ :

$$
\left\{\begin{array}{lll}
\Theta\left(r^{\prime}-r\right)=1 & \text { if } & r^{\prime}>r \\
\Theta\left(r^{\prime}-r\right)=0 & \text { if } & r^{\prime}<r
\end{array}\right.
$$

An index referring to the interfaces crossed, and subscripting the position vector, is then defined such that:

$$
\left|\overrightarrow{r_{k}}\right|<\left|\overrightarrow{r_{k+1}}\right|
$$

The difference between Heaviside functions allows us to construct a function which is equal to 1 between $\overrightarrow{r_{k}}$ and $\overrightarrow{r_{k+1}}$, i.e., in the medium $k$ :

[^150]\[

\left\{$$
\begin{array}{lll}
\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)=1 & \text { if } & \overrightarrow{r_{k}}<\vec{r}<\overrightarrow{r_{k+1}} \\
\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)=0 & \text { otherwise }
\end{array}
$$\right.
\]

The steady-state integro-differential equation can then be written in the discrete form ${ }^{18}$ :

$$
\begin{aligned}
& \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\sum_{k}\left(\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)\right) \Sigma_{t}^{k} \Phi(\vec{r}, \vec{\Omega}) \\
& \quad=S(\vec{r}, \vec{\Omega})+\sum_{k}\left(\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)\right) \int_{\Omega^{\prime}} d \vec{\Omega}^{\prime} \Sigma_{S}^{k} P_{k}\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

If a particular region $k^{\prime}$ is chosen, and its contribution to the left of the $=\operatorname{sign}$ is kept while the other contributions are moved to the right, the previous equation becomes:

$$
\begin{aligned}
& \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\left(\Theta\left(\overrightarrow{r_{k^{\prime}+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k^{\prime}}}-\vec{r}\right)\right) \Sigma_{t}^{k^{\prime}} \Phi(\vec{r}, \vec{\Omega}) \\
& = \\
& S(\vec{r}, \vec{\Omega})+\sum_{k}\left(\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)\right) \int_{\vec{\Omega}} d \vec{\Omega}^{\prime} \Sigma_{S}^{k} P_{k}\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi(\vec{r}, \vec{\Omega}) \\
& \quad-\sum_{k \neq k^{\prime}}\left(\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)\right) \Sigma_{t}^{k} \Phi(\vec{r}, \vec{\Omega})
\end{aligned}
$$

Using the following property of the Heaviside function:

$$
\Theta\left(\overrightarrow{r_{k^{\prime}+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k^{\prime}}}-\vec{r}\right)=1-\left[\Theta\left(\vec{r}-\overrightarrow{r_{k^{\prime}+1}}\right)+\Theta\left(\overrightarrow{r_{k^{\prime}}}-\vec{r}\right)\right]
$$

the preceding equation is transformed by moving all the Heaviside terms to the right:

$$
\begin{align*}
\vec{\Omega} \cdot \overrightarrow{g r a d} & \\
& \vec{r}, \vec{\Omega})+\Sigma_{t}^{k^{\prime}} \Phi(\vec{r}, \vec{\Omega}) \\
= & S(\vec{r}, \vec{\Omega})+\sum_{k}\left(\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)\right) \int_{\vec{\Omega}} \Sigma_{S}^{k} P_{k}\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi(\vec{r}, \vec{\Omega}) \\
& -\sum_{k \neq k^{\prime}}\left(\Theta\left(\overrightarrow{r_{k+1}}-\vec{r}\right)-\Theta\left(\overrightarrow{r_{k}}-\vec{r}\right)\right) \Sigma_{t}^{k} \Phi(\vec{r}, \vec{\Omega})  \tag{8.28}\\
& +\left(\Theta\left(\vec{r}-\overrightarrow{r_{k^{\prime}+1}}\right)+h \Theta\left(\overrightarrow{r_{k^{\prime}}}-\vec{r}\right)\right) \Sigma_{t}^{k^{\prime}} \Phi(\vec{r}, \vec{\Omega})
\end{align*}
$$

[^151]Let us define a Green's function $g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right)$ depending on the tiling of the space, and which satisfies the previous equation, by replacing the term on the right by the product of Dirac ${ }^{19}$ delta functions of space and direction $\delta\left(\vec{r}-\overrightarrow{r^{\prime}}\right) \delta\left(\vec{\Omega}-\vec{\Omega}^{\prime}\right)$, and which corresponds to the same boundary conditions imposed:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right)+\Sigma_{t}^{k^{\prime}} g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right)=\delta\left(\vec{r}-\overrightarrow{r^{\prime}}\right) \delta\left(\vec{\Omega}-\overrightarrow{\Omega^{\prime}}\right)
$$

$g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \vec{\Omega}^{\prime}\right)$ physically represents the flux at the point $\vec{r}$ in the direction $\vec{\Omega}$ created by a unit source (one neutron per second per unit solid angle) at $\overrightarrow{r^{\prime}}$ in the direction $\overrightarrow{\Omega^{\prime}}$ and emitting its neutrons in the medium having the same properties as the region $k^{\prime}$. In this medium referred to as first-flight-which is a concept already touched upon-each collision, be it absorption or scattering, removes the neutron from the considered neutron population, since the probability $\Sigma_{t}^{k^{\prime}}$ of removal of the neutron in the Green's function equation corresponds to the total cross section of the region $k^{\prime}$. In this way, a neutron contributes to the flux at the point $\vec{r}$ in this approach only if it has not undergone any collision in its path since the source. If the lethargy is considered, since the neutron has to not collide at all since the point source, its lethargy remains unchanged. The Green's function including the energy aspect is thus the product of the Green's function of space by a Dirac delta function of lethargy:

$$
g_{k}\left(\vec{r}, \vec{\Omega}, u, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}, u^{\prime}\right)=g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) \delta\left(u-u^{\prime}\right)
$$

The function $g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right)$ is used to integrate Eq. 8.28 and obtain:

$$
\Phi(\vec{r}, \vec{\Omega})=\iint_{\vec{r}} g_{\vec{\Omega}}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right)\left[\begin{array}{c}
S(\vec{r}, \vec{\Omega})+\sum_{k}\left(\Theta\left(\overrightarrow{r_{k+1}}-\overrightarrow{r^{\prime}}\right)-\Theta\left(\overrightarrow{r_{k}}-\overrightarrow{r^{\prime}}\right)\right) \int_{\vec{\Omega}} \sum_{s}^{k} P_{k}\left(\overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) \\
-\sum_{k \neq k^{\prime}}\left(\Theta\left(\overrightarrow{r_{k+1}}-\overrightarrow{r^{\prime}}\right)-\Theta\left(\overrightarrow{r_{k}}-\overrightarrow{r^{\prime}}\right)\right) \Sigma_{t}^{k_{t}^{k}} \Phi\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) \\
+\left(\Theta\left(\overrightarrow{r^{\prime}}-\overrightarrow{r_{k+1}}\right)+\Theta\left(\overrightarrow{r_{k^{\prime}}}-\overrightarrow{r^{\prime}}\right)\right) \Sigma_{t}^{\prime} \Phi\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right)
\end{array}\right]
$$

The integration over $\overrightarrow{r^{\prime}}$ is simplified by the fact that $\Theta\left(\overrightarrow{r_{k+1}}-\overrightarrow{r^{\prime}}\right)-\Theta\left(\overrightarrow{r_{k}}-\overrightarrow{r^{\prime}}\right)$ is 1 only between $\left|\overrightarrow{r_{k}}\right|$ and $\left|\overrightarrow{r_{k+1}}\right|$, and that $\Theta\left(\overrightarrow{r^{\prime}}-\overrightarrow{r_{k+1}}\right)+\Theta\left(\overrightarrow{r_{k^{\prime}}}-\overrightarrow{r^{\prime}}\right)$ is 0 between the same limits and 1 elsewhere, from which we obtain:

[^152]\[

$$
\begin{align*}
\Phi(\vec{r}, \vec{\Omega})= & \int_{r^{\prime}} d \overrightarrow{r^{\prime}} \int_{\vec{\Omega}^{\prime}} d \overrightarrow{\Omega^{\prime}} g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) S(\vec{r}, \vec{\Omega}) \\
& +\sum_{k}\left(\Sigma_{t}^{k^{\prime}}-\Sigma_{t}^{k}\right) \int_{\overrightarrow{r^{\prime}} \in k} d \overrightarrow{r^{\prime}} \int_{\vec{\Omega}^{\prime}} d \overrightarrow{\Omega^{\prime}} g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) \Phi\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) \\
& +\sum_{k} \int_{\overrightarrow{r^{\prime} \in k}} d \overrightarrow{r^{\prime}} \int_{\overrightarrow{\Omega^{\prime}}} d \overrightarrow{\Omega^{\prime}} g_{k}\left(\vec{r}, \vec{\Omega}, \overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) \int_{\Omega^{\prime \prime}} \Sigma_{s}^{k} P_{k}\left(\overrightarrow{\Omega^{\prime \prime}} \rightarrow \overrightarrow{\Omega^{\prime}}\right) \Phi\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime \prime}}\right) \tag{8.29}
\end{align*}
$$
\]

For the integration over angle, the flux, source, the differential scattering cross section and the Green's functions can be expressed in terms of a complete basis set of spherical harmonics. Because of the boundary conditions, the Green's functions can depend on both directions $\vec{\Omega}$ and $\vec{\Omega}^{\prime}$, and not only on their scalar product, which makes the expressions obtained more complex. If the space considered is infinite, the Green's function acts as a double Dirac delta function in direction, i.e., $\delta\left(\vec{\Omega}-\left(\vec{r}-\overrightarrow{r^{\prime}}\right)\right) \delta\left(\vec{\Omega}-\vec{\Omega}^{\prime}\right)$, which means that in the absence of scattering in the computation of the Green's function, only the neutrons emitted in the direction $\vec{\Omega}$ and along the vector $\left(\vec{r}-\overrightarrow{r^{\prime}}\right)$ contribute to the flux $\Phi(\vec{r}, \vec{\Omega})$. Substituting for the expansions in spherical harmonics ${ }^{20}$ in Eq. 8.29 results in terms that are products of spherical harmonics-most of which will result in zero after integration over angle. Ultimately, the homogeneous Green's functions method serves to transform the integro-differential equation in an integral equation with a kernel that satisfies Green's equation. Rather than neglect the flux moments in the expansion, this method allows us to neglect only the products of high order moments of the Green's function and the flux moments. Another advantage is that once the Green's functions that depend only on the geometry, the exterior surface, the total cross section of the region $k$ and the boundary conditions set on the domain (and optionally the energy for a multi-group problem) have been determined, the flux for any heterogeneous medium can be calculated, given the same boundary curve and boundary conditions. While this method can be equivalent in precision to very high orders of $P_{n}$ or $S_{n}$ methods, it can however become costly when evaluated the Green's functions for unusual geometries, which requires the use of Monte Carlo codes. It should be noted that in the case of a heterogeneous plate, whether it be multiplying or under-multiplying, Kornreich and Ganapol have obtained elegant solutions, ${ }^{21}$ which use the Green's functions method.

[^153]
### 8.3 Integral Form of the Boltzmann Equation

(Soodak 1962, p112; Stacey 2001, p301; Meghreblian and Holmes 1960, p366)

### 8.3.1 Peierls Operator

A form of the Boltzmann equation where the flux appears in a differential (gradient) operator has previously been seen. However, it is possible to write this equation in the form of an integral operator called the Peierls operator (after the works of Sir Rudolph Peierls ${ }^{22}$ ).


The book on Sir Rudolph Peierls by Sabine Lee and a portrait of the scientist knighted by the Queen of England (The Marguet collection and Public domain)

[^154]This integral is particular suitable for a numerical method called collision probability method or $P_{i j}$ method, which will be addressed in the next chapter. The flux at $\vec{r}$ in the direction $\vec{\Omega}$ originates from neutrons having interacted at $\vec{r}-\ell \vec{\Omega}$ at time $t-\ell / v$, which took the direction $\vec{\Omega}$, and which have not been absorbed along the path on the straight-line $\ell$. The scattering collision rate of neutrons at the point $\vec{r}-\ell \vec{\Omega}$ which took the direction $\vec{\Omega}$ having come from direction $\vec{\Omega}^{\prime}$, is given by:

$$
\Sigma_{S}\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, v^{\prime} \rightarrow v\right) \Phi\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime}, v^{\prime}, t\right)
$$

The probability of the neutron being uncollided along the straight-line path $\ell$ is given by (Fig. 8.13):

$$
e^{\left(-\int_{0}^{\ell} \Sigma_{t}\left(\vec{r}-\ell^{\prime} \vec{\Omega}, v\right) d \ell^{\prime}\right)}
$$

The quantity:
Optical path: $\quad \overline{\Sigma_{t} \ell} \equiv \int_{0}^{\ell} \Sigma_{t}\left(\vec{r}-\ell^{\prime} \bar{\Omega}, v\right) d \ell^{\prime}$
is called the optical path even if it is dimensionless, because it is related to the distance travelled while uncollided. The optical path is sometimes denoted by $\tau$ or $\tilde{\Sigma_{t} R}$ in some reference textbooks. And it always arises in the transport equation in the form $e^{-\overline{\Sigma_{t} \ell}}$. The flux in the absence of a source is obtained by integrating the uncollided neutrons along the optical path $\overline{\Sigma_{t} \ell}$ over all the possible interaction points in space, all the speeds and all the incident angles of interaction:

Integral form of the Boltzmann equation in the absence of a source:

$$
\begin{equation*}
\Phi(\vec{r}, \vec{\Omega}, v, t)=\int_{0}^{\infty} d \ell \int_{4 \pi} d \overrightarrow{\Omega^{\prime}} \int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, v^{\prime} \rightarrow v\right) \Phi\left(\vec{r}-\ell \vec{\Omega}, \overrightarrow{\Omega^{\prime}}, v^{\prime}, t-\frac{\ell}{v}\right) e^{-\overline{\Sigma_{t}}} \tag{8.31}
\end{equation*}
$$

This equation is generally solved by assuming that the cross sections are independent of time or at least of the considered time step (slow transient

Fig. 8.13 Contribution to the flux at the point $\vec{r}$

diffusion
hypothesis). In the presence of isotropic fission sources (i.e., $\chi(v, \vec{\Omega})=\chi(v) /(4 \pi))$ and without external sources, the integral equation is written:

$$
\begin{aligned}
\Phi(\vec{r}, \vec{\Omega}, v, t)= & \chi(v) \int_{0}^{\infty} d \ell \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{0}^{\infty} d v^{\prime} v \Sigma_{f}\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime}, v^{\prime}\right) \Phi\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime}, v^{\prime}, t-\frac{\ell}{v}\right) e^{-\overline{\Sigma_{t} \ell}} \\
& +\int_{0}^{\infty} d \ell \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, v^{\prime} \rightarrow v\right) \Phi\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}^{\prime}, v^{\prime}, t-\frac{\ell}{v}\right) e^{-\overline{\Sigma_{\ell} \ell}}
\end{aligned}
$$

The notations can be simplified by introducing the neutron source $q(\vec{r}, \vec{\Omega}, v, t)$ which represents the integrate fission source (with a fission cross section $v \Sigma_{f}$ ), the integrated scattering sources and any other external sources $S(\vec{r}, \vec{\Omega}, v, t)$ :

$$
\Phi(\vec{r}, \vec{\Omega}, v, t)=\int_{0}^{\infty} d \ell q\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}, v, t-\frac{\ell}{v}\right) e^{-\overline{\Sigma_{t} \ell}}
$$

where:

$$
\begin{aligned}
q(\vec{r}, \vec{\Omega}, v, t)= & \chi(v) \int_{0}^{\infty} d \ell \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{0}^{\infty} d v^{\prime} v \Sigma_{f}\left(\vec{r}, \vec{\Omega}^{\prime}, v^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}, v^{\prime}, t\right) \\
& +\int_{0}^{\infty} d \ell \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, v^{\prime} \rightarrow v\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}, v^{\prime}, t\right) \\
& +S(\vec{r}, \vec{\Omega}, v, t)
\end{aligned}
$$

The Peierls operator $K[]$, which represents the attenuated transport of the collided neutrons and coupled sources, can now be used:

$$
\Phi(\vec{r}, \vec{\Omega}, v, t)=K[q]=\int_{0}^{\infty} d \ell q\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}, v, t-\frac{\ell}{v}\right) e^{-\overline{\Sigma_{t} \ell}}
$$

More precisely, if the operator $K[]$ acts on the source $q$, it is called the Peierls attenuation operator and if it acts on the flux $\Phi$, the Peierls collision operator, $H[\Phi] \equiv K[q]$.

If the medium is isotropic, the dependence of the fission cross sections on angle can be ignored. And the scattering cross section will only depend on the scalar product $\vec{\Omega} . \vec{\Omega}^{\prime}$, leading to $\Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}, v, t\right)=\Sigma_{s}\left(\vec{r}, \vec{\Omega} . \vec{\Omega}^{\prime}, v, t\right)$. The total cross section takes into account the scattering cross section. This hypothesis is generally valid in reactors if the regions are properly homogenized.

If the scattering is isotropic, we can write $\Sigma_{s}(\vec{r}, \vec{\Omega}, v, t)=\Sigma_{s}(\vec{r}, v, t) /(4 \pi)$. This is the case of most materials used in reactors with the notable exception of water, which shows a strong anisotropy.

If the flux is isotropic, we can write $\Phi(\vec{r}, \vec{\Omega}, v, t)=\Phi(\vec{r}, v, t) /(4 \pi)$. This is rarely true, except in very simple cases of point sources in an infinite medium for example, or in huge approximations of reality.

The delayed neutrons, which can be emitted up to several seconds/minutes after the fission by the fission products, can be taken into account in the integral form through the source term via a delay between absorption and emission.

The scalar flux is obtained by integrating the angular flux over $4 \pi$ steradians:

$$
\Phi(\vec{r}, v, t)=\int_{4 \pi} \Phi(\vec{r}, \vec{\Omega}, v, t) d \vec{\Omega}=\int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} d \ell q\left(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}, v, t-\frac{\ell}{v}\right) e^{-\overline{\Sigma_{t} \ell}}
$$

which will be changed to a volume integral over the whole reactor by noticing that for $\vec{r}^{\prime}=\vec{r}-\ell \vec{\Omega}$, the volume element around $\vec{r}^{\prime}$ is $d^{3} r^{\prime}=\ell^{2} d \ell d \vec{\Omega}$ (Bussac and Reuss $1985, \mathrm{p} 81$ ). This allows us to remove $d \vec{\Omega}$ in the case where the scattering and the sources are isotropic ( $4 \pi$ term appears instead). Hence, using:

$$
\Phi\left(\vec{r}, v^{\prime}, t-\frac{\ell}{v}\right)=\int_{4 \pi} \Phi\left(\vec{r}, v^{\prime}, t-\frac{\ell}{v}\right) d \vec{\Omega}
$$

we find (Bussac and Reuss 1985, p82; Duderstadt and Hamilton 1976, p133):

$$
\begin{aligned}
\Phi(\vec{r}, v, t) & =\int_{V} d^{3} r^{\prime} q\left(\vec{r}^{\prime}, v, t-\frac{\ell}{v}\right) \frac{e^{-\overline{\Sigma_{t} \ell}}}{4 \pi \ell^{2}} \\
& =\int_{V} d^{3} r^{\prime} \frac{-\overline{\Sigma_{t} \ell}}{4 \pi \ell^{2}}\left[\begin{array}{l}
\chi(v) \int_{0}^{\infty} d v^{\prime} v \Sigma_{f}\left(\vec{r}^{\prime}, v^{\prime}\right) \Phi\left(\vec{r}^{\prime}, v^{\prime}, t-\frac{\ell}{v}\right) \\
\left.+\int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}^{\prime}, v^{\prime} \rightarrow v\right) \Phi\left(\vec{r}^{\prime}, v^{\prime}, t-\frac{\ell}{v}\right)+S\left(\vec{r}^{\prime}, v, t-\frac{\ell}{v}\right)\right]
\end{array}\right.
\end{aligned}
$$

We then talk of a volume integral form (isotropic), the general form of which will be discussed in the section below.

### 8.3.2 The Volume Integral Form

It is often more practical to numerically solve the integral form by adding an integration over volume. The solution for the flux is then written:

$$
\begin{aligned}
\Phi(\vec{r}, v, \vec{\Omega})= & \int_{V} d^{3} r^{\prime} \int_{4 \pi} d \overrightarrow{\Omega^{\prime}} \frac{\left.e^{-\overrightarrow{\Sigma_{r} \ell}\left(\vec{r},\left|\vec{r}-\overrightarrow{r^{\prime}},\right|, \frac{\overrightarrow{r-r}}{\vec{r}-r^{\prime}}, v\right.}\right)}{\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} \delta_{2}\left(\vec{\Omega}, \overrightarrow{\Omega^{\prime}}\right) \delta_{2}\left(\frac{\vec{r}-\overrightarrow{r^{\prime}}}{\left|\vec{r}-\overrightarrow{r^{\prime}}\right|}, \overrightarrow{\Omega^{\prime}}\right) \\
& {\left[\int_{0}^{\infty} d v^{\prime} \int_{4 \pi} d \overrightarrow{\Omega^{\prime}} \Sigma_{s}\left(\overrightarrow{r^{\prime}}, v^{\prime} \rightarrow v, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\overrightarrow{r^{\prime}}, v^{\prime}, \overrightarrow{\Omega^{\prime}}\right)+S\left(\overrightarrow{r^{\prime}}, v, \overrightarrow{\Omega^{\prime}}\right)\right] }
\end{aligned}
$$

where $\overline{\Sigma_{t} \ell}(\vec{r}, \ell, \vec{\Omega}, v)=\int_{0}^{\ell} d \ell^{\prime} \Sigma_{t}\left(\vec{r}-\ell^{\prime} \vec{\Omega}, v\right)$ is the optical path. The integration over angle $\vec{\Omega}=\left(\vec{r}-\overrightarrow{r^{\prime}}\right) /\left|\vec{r}-\overrightarrow{r^{\prime}}\right|$ of the angular flux serves to remove the Dirac delta function over angle and obtain the scalar flux:

Volume integral form:

$$
\begin{align*}
\Phi(\vec{r}, v)= & \int_{4 \pi} d \vec{\Omega} \Phi(\vec{r}, v, \vec{\Omega}) \int_{V} d^{3} r^{\prime} \frac{e^{-\overline{\Sigma_{\ell}}\left(\vec{r},\left|\vec{r}-\overrightarrow{r^{\prime}}\right|, \vec{\Omega}, v\right)}}{\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} \\
& \times\left[\int_{0}^{\infty} d v^{\prime} \int_{4 \pi} d \overrightarrow{\Omega^{\prime}} \Sigma_{s}\left(\overrightarrow{r^{\prime}}, v^{\prime} \rightarrow v, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\overrightarrow{r^{\prime}}, v^{\prime}, \overrightarrow{\Omega^{\prime}}\right)+S\left(\overrightarrow{r^{\prime}}, v, \vec{\Omega}\right)\right] \tag{8.32}
\end{align*}
$$

Recall that the source term comprises the fission sources and the external sources. In numerous cases, it is assumed that the scattering is linearly anisotropic, i.e., that the scattering cross section is a linear function of the cosine of the deviation angle, denoted by $\mu_{0}=\vec{\Omega} . \overrightarrow{\Omega^{\prime}}$ and expressed in terms of an expansion in Legendre polynomials:

$$
\Sigma_{s}\left(\vec{r}, v^{\prime} \rightarrow v, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right)=\frac{1}{4 \pi}\left[\Sigma_{s, 0}\left(\vec{r}, v^{\prime} \rightarrow v\right)+3 \mu_{0} \Sigma_{s, 1}\left(\vec{r}, v^{\prime} \rightarrow v\right)\right]
$$

For isotropic scattering and source, the scalar flux, after integration over the speed, is given by:

$$
\Phi(\vec{r})=\int_{V} d^{3} r \frac{e^{-\overline{\Sigma_{r} \ell}\left(\vec{r},\left|\vec{r}-\overrightarrow{r^{\prime}}\right|\right)}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}}\left(\Sigma_{s, 0}\left(\overrightarrow{r^{\prime}}\right) \Phi\left(\overrightarrow{r^{\prime}}\right)+S\left(\overrightarrow{r^{\prime}}\right)\right)
$$

The approximation to the scattering cross section is often called the $B_{n}$ approximation, where $n$ is the order to which the scattering cross section is expanded. Hence, in the previous equation, it is a $B_{1}$ approximation. The source can also be written in the form:

$$
S(\vec{r}, v, \vec{\Omega})=\frac{1}{4 \pi}\left[S_{0}(\vec{r}, v)+3 \vec{\Omega} \cdot \overrightarrow{S_{1}}(\vec{r}, v)\right]
$$

where

$$
\left\{\begin{array}{c}
S_{0}(\vec{r}, v)=\int_{4 \pi} d \vec{\Omega} S(\vec{r}, v, \vec{\Omega}) \quad S_{1}(\vec{r}, v)=\int_{4 \pi} d \vec{\Omega} \vec{\Omega} S(\vec{r}, v, \vec{\Omega}) \\
\Sigma_{s, 0}\left(\vec{r}, v^{\prime} \rightarrow v\right)=\int_{\mu_{0}} d \mu_{0} \Sigma_{s}\left(\vec{r}, v^{\prime} \rightarrow v, \mu_{0}\right) \quad \Sigma_{s, 1}\left(\vec{r}, v^{\prime} \rightarrow v\right)=\int_{\mu_{0}} d \mu_{0} \mu_{0} \Sigma_{s}\left(\vec{r}, v^{\prime} \rightarrow v, \mu_{0}\right)
\end{array}\right.
$$

The neutron angular current (vector) is then defined as:

$$
\vec{J}(\vec{r}, v, \vec{\Omega})=\vec{\Omega} \Phi(\vec{r}, v, \vec{\Omega})
$$

where the following integration over angle gives the scalar or integrated current:

$$
\vec{J}(\vec{r}, v)=\int_{4 \pi} d \vec{\Omega} \vec{\Omega} \Phi(\vec{r}, v, \vec{\Omega})
$$

### 8.3.3 The First Collision Probability

(Reuss 1985, p181; Stamm'ler and Abbate 1983, p115)

### 8.3.3.1 Definition of the First Collision Probability

The collision probability method is the oldest method to solve the integral form of the transport equation. ${ }^{23,24}$ It is based on the computation of the probability of first collision when considering two zones of the reactor. It is a costly method when it comes to computational time, and is in fact generally used for one or two-dimensional geometries (as is the case in the French APOLLO2 code from the $C E A$ ), and very rarely for three-dimensional ones.

It consists in simplifying Peierls operator through a partitioning of the space and assumes a $B_{0}$ approximation, meaning that the scattering and sources are isotropic. A problem where the energy has been integrated over will be examined in order to

[^155]simplify notation by eliminating the $E$ variable. The Peierls operator integrated over energy is written as:
$$
\Phi(\vec{r})=\int d \overrightarrow{r^{\prime}} \frac{e^{-\overline{r_{t} \ell}\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right)
$$
where:
$$
q\left(\overrightarrow{r^{\prime}}\right)=\int_{0}^{\infty} d E\left[\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(\overrightarrow{r^{\prime}}, E^{\prime} \rightarrow E\right) \Phi\left(\overrightarrow{r^{\prime}}, E^{\prime}\right)+S\left(\overrightarrow{r^{\prime}}, E\right)\right] \Sigma_{s}\left(\overrightarrow{r^{\prime}}\right) \Phi\left(\overrightarrow{r^{\prime}}\right)+S\left(\overrightarrow{r^{\prime}}\right)
$$

Let $V_{i}$ represent a partitioning of the space into regions such that $V=\sum_{i=1}^{n} V_{i}$, an integration of the reaction rate is carried out over each of these:

$$
\begin{align*}
& \text { Evaluation of the total reaction rate: } \int_{V_{i}} d \vec{r} \Sigma_{t}(\vec{r}) \Phi(\vec{r}) \\
& \qquad \begin{array}{c}
\int_{V_{i}} d \vec{r} \Sigma_{t}(\vec{r}) \quad \int_{V=\sum_{j} V_{j}} d \overrightarrow{r^{\prime}} \frac{e^{-\overline{\Sigma_{t} \ell}\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right) \\
=\int_{V_{i}} d \vec{r} \Sigma_{t}(\vec{r}) \sum_{j} \int_{V_{j}} d \overrightarrow{r^{\prime}} \frac{e^{-\overline{\Sigma_{t} \ell}\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right)
\end{array}
\end{align*}
$$

The following volume-averaged variables are then used:

$$
\Phi_{i}=\frac{\int_{V_{i}} d \vec{r} \Phi(\vec{r})}{V_{i}}, q_{i}=\frac{\int_{V_{i}} d \vec{r} q(\vec{r})}{V_{i}}, S_{i}=\frac{\int_{V_{i}} d \vec{r} S(\vec{r})}{V_{i}} \text { et } \quad \Sigma_{t}^{i}=\frac{\int_{V_{i}} d \vec{r} \Sigma_{t}(\vec{r}) \Phi(\vec{r})}{\Phi_{i}}
$$

and the probability of a neutron emitted from the volume $V_{i}$ to undergo its first collision in the volume $V_{j}$ is given by:
$\tilde{P}_{i j}=\tilde{P}_{i \rightarrow j} \equiv \frac{\int_{V_{j}} d \vec{r} \Sigma_{t}(\vec{r}) \int_{V_{i}} d \overrightarrow{\left.r^{\prime} e^{-\overline{\varepsilon_{t}}( }\right) \frac{\vec{r}, \overrightarrow{r^{\prime}}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}}} q\left(\overrightarrow{r^{\prime}}\right)}{\int_{V_{i}} d \overrightarrow{r^{\prime}} q\left(\overrightarrow{r^{\prime}}\right)}=\frac{\int_{V_{j}} d \vec{r} \Sigma_{t}(\vec{r}) \int_{V_{i}} d \overrightarrow{r^{\prime} \frac{e^{-\overline{\Sigma_{t} t}}\left(\vec{r}, \overrightarrow{r^{\prime}}\right.}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right)}}{V_{i} q_{i}}$

If the density $q$ is constant in the elementary volumes, we define ${ }^{25}$ :

$$
P_{i \rightarrow j}=P_{i j} \equiv \frac{\int_{V_{j}} d \vec{r} \Sigma_{t}(\vec{r}) \int_{V_{i}} d \overrightarrow{r^{\prime}} \frac{\overrightarrow{e^{-\overline{z_{t}}( }\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}}}{V_{i}}
$$

With these defined variables, Eq. 8.33 is written:
Flux equations given by the $P_{i j}$ method:

$$
\begin{equation*}
\Sigma_{t}^{i} \Phi_{i} V_{i}=\sum_{j=1}^{n} P_{j i} q_{j} V_{j} \quad \text { for } \quad i=1 \text { to } n \tag{8.34}
\end{equation*}
$$

and also:

$$
q_{j}=\Sigma_{s}^{j} \Phi_{j}+S_{j}=\left(\Sigma_{s}^{j}+\nu \Sigma_{f}^{j}\right) \Phi_{j}+S_{j}^{\text {autonomous }}
$$

This second equation serves as a reminder that the source $S_{j}$ as it is defined, contains the fission sources. Some authors prefer using the reduced collision probability or transmission probability (Stacey 2001, p320, denoted $T_{j \leftarrow i}$ ), which does not contain the total cross section and which is divided by the considered volume:

$$
p_{i j}=\frac{\int_{V_{j}} d \vec{r} \int_{V_{i}} d \overrightarrow{r^{\prime}} \frac{\overrightarrow{-\overline{\bar{z}_{t}}}\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}}}{V_{j}}
$$

These reduced probabilities satisfy:

$$
\left\{\begin{array} { l } 
{ V _ { i } p _ { j i } = V _ { j } p _ { i j } } \\
{ p _ { i j } = \frac { \Sigma _ { t } ^ { j } p _ { i j } V _ { j } } { V _ { i } } }
\end{array} \left\{\begin{array}{l}
V_{j} \Phi_{j}=\sum_{i=1}^{n} V_{j} p_{i j} q_{i} \\
\Phi_{j}=\sum_{i=1}^{n} p_{i j} q_{i}
\end{array}\right.\right.
$$

The French code APOLLO2 itself uses volume reduced collision probabilities defined by:

[^156]$$
p_{i j}^{A p o}=\frac{V_{i} P_{i j}}{\Sigma_{t}^{j}} .
$$

These have the advantage of remaining finite even if the medium is a vacuum, and allows us to write the reciprocity relations in the very mnemonic form:

$$
p_{j i}^{A p o}=p_{i j}^{A p o}
$$

If the $P_{i j}$ are known, the method leads to resolving a linear system coupling the fluxes from different regions. This calculation assumes a flat flux (average value) in the regions. The precision can be improved by assuming a linear flux in space (in between two interfaces). The reciprocal probabilities $P_{i j}$ are related to the probabilities $P_{i j}$ by the reciprocity relation:

Reciprocity of the $P_{i j}: \Sigma_{t}^{j} P_{j i} V_{j}=\Sigma_{t}^{i} P_{i j} V_{i}$
The reciprocity of the $P_{i j}$ implies that only $n(n+1) / 2$ probabilities need to be calculated. If there is no leakage from the medium, it entails that a neutron definitely has to interact somewhere-which is represented by the normalization equation:

Normalization equation for the $P_{i j}$ in an infinite medium: $\forall i, \quad \sum_{j=1}^{n} P_{i j}=1$

It results from this conservation law that only $n(n-1) / 2$ probabilities have to be computed in an infinite medium (though still $n(n+1) / 2$ in a finite medium). For large domain problems, these computations are still expensive. The probability that a neutron escapes uncollided through a surface $S_{i}$ around a volume $V_{i}$ is related to the collision probability in that volume through:

$$
P_{i S_{i}}+P_{i i}=1
$$

Thanks to the reciprocity theorem, the probability that a neutron entering through the surface $S_{i}$ interacts in $V_{i}$ is given by:

$$
\begin{equation*}
P_{S_{i} i}=\frac{4 V_{i}}{S_{i}} \Sigma_{t}^{i} P_{i S_{i}} \tag{8.37}
\end{equation*}
$$

This result is particular simple to prove because of the Dirac's chord method, which will be looked at in detail later. More generally, the probability of reaching uncollided the exterior surface $S$ of a volume $V$ (sum of the volumes $V_{i}$ ) is
complementary to the probabilities of interaction in the domain. This translates to the fact that the neutron is either absorbed or leaks out of $V$ through its surface:

$$
\sum_{j=1}^{n} P_{i j}+P_{i S}=1
$$

This probability can be calculated by integrating the neutrons reaching any point of the surface uncollided:

$$
P_{i S}=\frac{\int_{V_{i}} d \overrightarrow{r^{\prime}} \int_{S} d S \vec{\Omega} \cdot \vec{n} \frac{e^{-\overrightarrow{\varepsilon_{t} \ell}\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}}{4 \pi\left|\overrightarrow{r_{S}}-r^{\prime}\right|^{2}}}{V_{i}} \text { for } \quad \vec{\Omega} . \vec{n}>0
$$

However, this result is more easily obtained every $P_{i j}$ value has already been calculated, using $P_{i S}=1-\sum_{j=1}^{n} P_{i j}$. Also, by extension, we can define the probability that a neutron entering through the surface $S$ undergoes its first collision in the volume $V_{i}$, or the probability that a neutron goes through the volume $V$ from end to end to reach the surface $S$ on the opposite side uncollided. Because these are complementary, we can write:

$$
\sum_{i=1}^{n} P_{S i}+P_{S S}=1
$$

The result of Eq. 8.37 giving the probability $P_{i S}$, the reciprocal of $P_{S i}$, can be generalized at the surface of the complete volume $V$ :

$$
P_{S i}=\frac{4 V_{i}}{S} \Sigma_{t}^{i} P_{i S}
$$

### 8.3.3.2 Calculating First Collision Probabilities

(Silvennoinen 1976, p166; Stamm'ler and Abbate 1983, p119)
The first collision probability method requires the calculation of the probabilities of first collision in the actual geometry of the reactor. Let us first consider a one-dimensional problem with a homogeneous medium of total cross section $\Sigma_{t}$ where we are looking for the probability of reaching uncollided the point $r$ on a cylindrical element for neutrons emitted from an isotropic line source placed on the axis of said cylinder (Fig. 8.14). Assuming the neutron is emitted with an angle $\theta$, this probability will be denoted by $p(r, \theta)$.

Fig. 8.14 Probability of reaching the point $r$ on the cylindrical elementnotations


The optical path separating the point source at the origin and the point $P$ on the cylinder is given by $\Sigma_{t} r / \sin \theta$. The probability of reaching the point $P$ for the angle $\theta$ is:

$$
p(r, \theta)=e^{-\sum_{t \cdot \frac{r}{\sin \theta}}}
$$

The probability for a neutron to be emitted in the differential angular element $d \theta$ from the origin $O$ to the point $P$ is proportional to the solid angle $\sin \theta d \theta d \varphi$ because of the nature of the isotropic emission from each point source along the line. The probability of reaching the edge of the cylindrical element can be deduced through an integration, where the point source is moved along the line source $(\theta \in] 0, \pi / 2]$, zero-angle for the points $O$ at infinite, right angle for the point $O$ obtained by projection of the point $P$ on the line) (Stacey 2001, p310, proved this result by integrating the point source kernel):

$$
p(r)=\frac{\int_{0}^{2 \pi} d \varphi \int_{0}^{\frac{\pi}{2}} e^{-\Sigma_{\left(\frac{r}{\sin \theta} \theta\right.}} \sin \theta d \theta}{\int_{0}^{2 \pi} d \varphi \int_{0}^{\frac{\pi}{2}} \sin \theta d \theta}=K i_{2}\left(\Sigma_{t} r\right)
$$

where a Bickley-Nayler function of order 2 has been used, i.e., $K i_{2}$, the general form (Lewis and Miller 1993) of which is given by:

$$
K i_{n}(x)=\int_{0}^{\frac{\pi}{2}}(\sin \theta)^{n-1} e^{-\frac{x}{\sin \theta}} d \theta=\int_{0}^{\frac{\pi}{2}}(\cos \theta)^{n-1} e^{-\frac{x}{\cos \theta}} d \theta
$$

These functions, which are very much analogous to modified Bessel functions $K_{n}$, have been numerically ${ }^{26}$ tabulated from 1935 by W.G. Bickley ${ }^{27}$ and John Nayler. ${ }^{28}$ In the case of a 2D geometry extruded in the $z$ direction (Fig. 8.15), a ray tracing method is used, since it is very rare to have a simple enough geometry that an analytical integration is possible. This method consists of mentally tracing at an angle $\theta$, a network of parallel lines (rays), which go through the surfaces of interest, and then combining the probabilities of non-collision (escape). The probability that a neutron, emitted at the point $x$ (belonging to the segment $\left[d_{i}\right]$ ) in the direction $\theta$ going through the volumes $V_{i}$ and $V_{j}$, undergoes its first collision in the volume $V_{j}$ is given by:

$$
p\left(x \in\left[d_{i}\right] \rightarrow \forall x_{j} \in\left[d_{j}\right] \theta\right)=K i_{2}\left(\Sigma_{t}^{j}\left(d_{j}-x\right)\right) K i_{2}\left(\overline{\Sigma_{t} d_{i}^{j}}\right)\left(1-K i_{2}\left(\Sigma_{t}^{j} d_{j}\right)\right)
$$

The primary rationale for using the functions $\mathrm{Ki}_{2}$ —which were encountered when calculating the escape probability from an isotropic line source-is noticing that here, the escape probability of a neutron emitted from an isotropic line source along the $z$ axis and placed at the abscissa $x$ on the segment $\left[d_{i}\right]$ has to be computed. The forms of the successive probabilities explain the product of the three independent probabilities. The origin of the $x$ axis is the point of entry in the volume $V_{i}$, and $\left(1-K i_{2}\left(\Sigma_{t}^{j} d_{j}\right)\right)$ is the probability of interaction in the volume $V_{j}$ from the definition of $K i_{2}\left(\Sigma_{t}^{j} d_{j}\right)$.

The medium in between $V_{i}$ and $V_{j}$ is supposed to have an optical path of $\overline{\Sigma_{t} d_{i}^{j}}$ which is zero in the case of a vacuum, in which case the probability of crossing the distance $d_{i}^{j}$ is 1 . The overall probability $p_{i j}$ is obtained by averaging the probabilities for each ray:

[^157]

Fig. 8.15 Ray tracing in $2 D$ geometry

$$
P_{i j}=\frac{\int_{0}^{2 \pi} d \theta \int_{0}^{Y(\theta)} d y \int_{0}^{d_{i}(Y)} p\left(x \in\left[d_{i}\right] \rightarrow \forall x_{j} \in\left[d_{j}\right] \theta\right) d x}{\int_{0}^{2 \pi} d \theta \int_{0}^{Y} d y \int_{0}^{d_{i}(Y)} d x}
$$

The result below, where the integral of a Bickley-Nayler function is said function of the next order, will be used:

$$
K i_{n}(x)=\int_{x}^{+\infty} K i_{n-1}(y) d y
$$

to obtain $K i_{3}$ functions after integration, since:

$$
\int_{0}^{d} K i_{2}(x) d x=K i_{3}(0)-K i_{3}(d)
$$

The probability that a neutron undergoes a collision in volume $V_{i}$ where it is emitted from, is:

$$
P_{i j}=\frac{\int_{0}^{2 \pi} d \theta \int_{0}^{Y(\theta)} d y \int_{0}^{d_{i}(Y)}\left(1-K i_{2}\left(\Sigma_{t}^{i}\left(d_{i}-x\right)\right)\right) d x}{2 \pi V_{i}}
$$

Hence, the computation of the $P_{i j}$ can be extended to $2 D$ (Stacey 2001, p313; Stamm'ler and Abbate 1983, p120), or even $3 D,{ }^{29}$ starting from the calculations done in $1 D$, albeit for the more or less tedious integrations. However, the determination of the ray tracing will be more and more expensive (searching for intersections and tangent planes for the integration limits). Hence, the $P_{i j}$ method is rarely used in $3 D$.

### 8.3.3.3 Dirac's Chord Method

(Duderstadt and Martin 1979)


Paul Dirac (1902-1984) was a British physicist and mathematician who postulated the existence of antimatter (positron of Dirac), which was later confirmed experimentally. Nobel Laureate in physics in 1933, he is also credited with very innovative mathematical concepts. (Public domain)

Consider a convex volume $V$ of any shape, containing a uniform distribution of neutrons from an isotropic source $S_{0}$. The number of uncollided neutrons coming from a volume element $d \vec{r}=d^{3} r$, and escaping from a surface element $d S$ surrounding the volume can be calculated as follows:

$$
\frac{d n}{d t}\left(\vec{r} \rightarrow \overrightarrow{r_{S}}\right)=\frac{S_{0}}{4 \pi} e^{-\Sigma_{t}\left|\overrightarrow{r_{S}}-\vec{r}\right|} d \vec{r} d \vec{\Omega}
$$

By integrating over contributions from the whole volume, i.e., over each element $d \vec{r}$, and then over the surface, the escape rate of neutrons through the surface $S$ is obtained (Fig. 8.16):

[^158]

Fig. 8.16 Escape from a volume

$$
\frac{d n}{d t}\left(V \rightarrow \overrightarrow{r_{S}}\right)=\frac{S_{0}}{4 \pi} \int_{\vec{r} \in V} \int_{\overrightarrow{r_{S}} \in S} e^{-\Sigma_{t}\left|\overrightarrow{r_{S}}-\vec{r}\right|} d \vec{r} d \vec{\Omega}
$$

Care should be taken if the volume is not convex. Indeed, we can then have $\vec{\Omega} \cdot \vec{n}<0$, which effectively translates to particles re-entering the volume, from other parts of it. The number of neutrons emitted in the volume being $S_{0} V$, we can deduce the probability of escaping uncollided from the volume, i.e., the first-flight escape probability (Case et al. 1953, p17), which will be indexed using 0 , to differentiate it from escape after several collisions (the term transmission probability is sometimes used):

$$
P_{V S, 0}=\frac{\frac{S_{0}}{4 \pi} \int_{\vec{r} \in V} d \vec{r} \int_{\vec{r} \in S} e^{-\Sigma_{t}\left|\overrightarrow{r_{S}}-\vec{r}\right|} d \vec{\Omega}}{S_{0} V}=\frac{1}{4 \pi V} \int_{\vec{r} \in V} d \vec{r} \int_{\vec{r} \in S} e^{-\Sigma_{t}\left|\overrightarrow{r_{s}}-\vec{r}\right|} d \vec{\Omega}
$$

To compute the spatial volume integral, the quantity $\vec{\Omega} \cdot \vec{n} d S d \ell$ will be chosen as volume element, where $\ell$ is the length along a path or chord joining two elements of opposite surface. This chord has a length $R_{\Omega}$ which depends on the direction. The volume integral will thus be transformed into an integral over the set of possible chords defined by the set of surface elements:

$$
\begin{align*}
P_{V S, 0} & =\frac{1}{4 \pi V} \int_{S} d S \int_{\ell=0}^{\ell=R_{\Omega}} \int_{\vec{\Omega}} d \vec{\Omega} e^{-\Sigma_{l} \ell} \vec{\Omega} \cdot \vec{n} \\
& =\frac{1}{4 \pi V \Sigma_{t}} \int_{S} d S \int_{\vec{\Omega}} d \vec{\Omega}\left(1-e^{-\Sigma_{l} R_{\Omega}}\right) \vec{\Omega} \cdot \vec{n} \tag{8.38}
\end{align*}
$$

Dirac then introduced the probability $p(R) d R$ that a chord has a given length $R$ in $d R$. The first moment of this probability gives the mean chord length $\langle R\rangle$, which allows us to use Cauchy's theorem relating mean chord length, volume and surface of a convex volume,

Cauchy's theorem for the mean chord length: $<R>=\int_{R_{\min }}^{R_{\max }} R p(R) d R=\frac{4 V}{S}$

The proof of this theorem through a neutronic approach (calculation of the absorption in a convex volume where the absorption cross section tends to zero) is given in (Dresner 1960, p60) and reproduced in (Spanier and Gelbard 1969, p152). The probability $p(R) d R$ is computed by an integration over the whole surface of the volume of the element $d \vec{\Omega} \vec{\Omega} \cdot \vec{n}$, expressed in the particular value of the desired chord $R$ :

$$
p(R) d R=\frac{<R>}{4 \pi V} \int_{R_{\Omega}=R} d S \int d \vec{\Omega} \vec{\Omega} \cdot \vec{n}
$$

By substituting this expression in Eq. 8.38, and simplifying, it is found:

$$
\begin{equation*}
P_{V S, 0}=\frac{1}{\left\langle R>\Sigma_{t}\right.} \int_{R_{\min }}^{R_{\max }}\left(1-e^{-\Sigma_{t} R}\right) p(R) d R \tag{8.40}
\end{equation*}
$$

### 8.3.4 1D Geometry

Historically, it is evident that it was one-dimensional geometries that were considered and solved first. In France, the code APOLLO1, which was integrated within a much larger framework of codes called NEPTUNE, ${ }^{30}$ was the crucible for theoretical developments of the water-moderated reactor physics department of the CEA/ Saclay. For a linearly anisotropic collision law, the solution for the flux from the integral transport equation is written:

[^159]\[

$$
\begin{aligned}
\Phi(\vec{r})= & \int d \overrightarrow{r^{\prime}} \frac{e^{-\overline{r_{\ell} \ell}\left(\vec{r}, \overrightarrow{r^{\prime}}\right)}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right) q\left(\overrightarrow{r^{\prime}}\right) \equiv \Sigma_{s}^{0}\left(\overrightarrow{r^{\prime}}\right) \Phi\left(\overrightarrow{r^{\prime}}\right)+S_{0}\left(\overrightarrow{r^{\prime}}\right) \\
& +\vec{\Omega} \cdot\left(\Sigma_{s}^{1}\left(\overrightarrow{r^{\prime}}\right) \vec{J}\left(\overrightarrow{r^{\prime}}\right)+\overrightarrow{S_{1}}\left(\overrightarrow{r^{\prime}}\right)\right)
\end{aligned}
$$
\]

In $1 D$ geometry characterized by the index $n(n=1$, slab, $n=2$, cylinder, $n=3$, sphere), the solution of the flux is written in condensed form (omitting the arrows on the position vectors for brevity's sake):

$$
\begin{aligned}
\Phi(r)= & \int_{r_{0}}^{r_{1}} G_{n}\left(r^{\prime}, r\right)\left(\Sigma_{s}^{0}\left(r^{\prime}\right) \Phi\left(r^{\prime}\right)+S_{0}\left(r^{\prime}\right)\right) r^{\prime n-1} d r^{\prime}+\int_{r_{0}}^{r_{1}} \widetilde{G_{n}}\left(r^{\prime}, r\right) \vec{\Omega} . \\
& \left(\Sigma_{s}^{1}\left(r^{\prime}\right) \vec{J}\left(r^{\prime}\right)+\overrightarrow{S_{1}}\left(r^{\prime}\right)\right) r^{\prime n-1} d r^{\prime}
\end{aligned}
$$

In this equation, $G_{n}\left(r^{\prime}, r\right)$ is the first-flight Green's function, i.e., the flux arising at $r$ from an isotropic unit source placed at $r^{\prime}$ and $\widetilde{G_{n}}\left(r^{\prime}, r\right)$ is the Green's function corresponding to an isotropic unit source multiplied by $\vec{\Omega}$. $\vec{n}$, where $\vec{n}$ is the normal to the plane tangent to the source. The balance equation in $l D$ geometry is given by:

$$
r^{n-1} J(r)=r_{0}^{n-1} J\left(r_{0}\right)+\int_{r_{0}}^{r}\left(S_{0}\left(r^{\prime}\right)-\Sigma_{a}\left(r^{\prime}\right) \Phi\left(r^{\prime}\right)\right) r^{\prime n-1} d r^{\prime}
$$

APOLLO1 had four approximations:

- Isotropic collision and flat flux: the medium is divided into $J$ regions and the reduced collision probabilities were defined for each energy group $g$
$p_{j i}^{g}=\frac{\varpi_{n}}{V_{i}} \int_{r_{i-1}}^{r_{i}} r^{n-1} d r \int_{r_{j-1}}^{r_{j}} G_{n}\left(r^{\prime}, r\right) r^{\prime n-1} d r^{\prime}$ where $\varpi_{n}$ is a geometric coefficient.
The flux is then obtained by summation:

$$
\Phi_{i}^{g}=\sum_{j=1}^{J} p_{j i}^{g}\left(\Sigma_{s, g \rightarrow g}^{0} \Phi_{j}^{g}+\sum_{g^{\prime}} \Sigma_{s, g^{\prime} \rightarrow g}^{0} \Phi_{j}^{g^{\prime}}+S_{j, g}^{0}\right)
$$

- Linear anisotropic collision and flat flux: the isotropic part is treated as before when the anisotropic part is introduced:

$$
\tilde{p}_{j i}^{g}=\frac{\varpi_{n}}{V_{i}} \int_{r_{i-1}}^{r_{i}} r^{n-1} d r \int_{r_{j-1}}^{r_{j}} \widetilde{G_{n}}\left(r^{\prime}, r\right) r^{\prime n-1} d r^{\prime}
$$

- Isotropic collision and linear flux: the flux is made linear in a region between two consecutive interfaces $j_{1}$ and $j_{2}$, by writing:

$$
\Phi_{i}(r)=\alpha(r) \Phi_{j_{1}}^{g}+\beta(r) \Phi_{j_{2}}^{g} \quad \text { for } r \in\left[j_{1}, j_{2}\right]
$$

where $\alpha(r)$ and $\beta(r)$ are independent polynomials. The new unknowns of the problem become the fluxes at the interfaces $\Phi_{j_{k}}^{g}$. A general form of the probabilities, $p_{j i k}^{g}$, is then used:

$$
\Phi_{i}^{g}=\sum_{j=1}^{J} \sum_{k=1}^{2} p_{j i k}^{g}\left(\Sigma_{s, g \rightarrow g}^{0} \Phi_{j_{k}}^{g}+\sum_{g^{\prime}} \Sigma_{s, g^{\prime} \rightarrow g}^{0} \Phi_{j_{k}}^{g^{\prime}}+S_{j, g}^{0}\right)
$$

- Linearly anisotropic flux and linear flux ${ }^{31}$ : the same method as before is used for the isotropic part while the anisotropic general form of the probabilities, $\tilde{p}_{j i k}^{g}$, is introduced.
$2 D$ calculations are now used instead of this historical $1 D$ approach, and this will be detailed further in Chap. 14.


### 8.3.5 Escape Probabilities

(Duderstadt and Hamilton 1976, p415)

### 8.3.5.1 Escape Probability from a Slab

In the case of a slab of thickness $a$ and infinite in the other dimensions, the mean chord is given by:

$$
<R>=2 a
$$

However, $\left\langle R^{2}\right\rangle=+\infty$ (Reuss 1985, p184). Noticing that (Fig. 8.17) $\cos ^{2}$ $\theta=1-a^{2} / R^{2}$ and $\mu=\cos \theta$, we obtain by differentiation:

[^160]Fig. 8.17 Slab with thickness $a$


$$
2 \cos \theta d(\cos \theta)=2 \mu d \mu=2 \frac{a^{2}}{R^{3}} d R
$$

where, since $d \vec{\Omega}=2 \pi d \mu$ and $\vec{\Omega} \cdot \vec{n}=-\cos \theta$, we can compute the probability $p(R)$ :

$$
p(R) d R=\frac{<R>}{4 \pi V} \int_{R_{\Omega}=R} d S \int d \vec{\Omega} \vec{\Omega} \cdot \vec{n}=\frac{1}{\pi S} S 2 \pi \mu d \mu=2 \mu d \mu=\frac{2 a^{2}}{R^{3}} d R
$$

By substituting this result in Eq. 8.40, we find, for an infinite slab:

$$
\begin{aligned}
P_{V S, 0} & =\frac{1}{<R>\Sigma_{t}} \int_{a}^{+\infty}\left(1-e^{-\Sigma_{t} R}\right) p(R) d R=\frac{1}{2 a \Sigma_{t}} \int_{a}^{+\infty} 2\left(1-e^{-\Sigma_{t} R}\right) \frac{a^{2}}{R^{3}} d R \\
& =\frac{1}{2 a \Sigma_{t}} \int_{1}^{+\infty} \frac{2}{y^{3}}\left(1-e^{-\Sigma_{t} a y}\right) d y
\end{aligned}
$$

where the exponential function $E_{3}\left(\Sigma_{t} a\right)=\int_{1}^{+\infty} \frac{1}{y^{3}} e^{-\Sigma_{t} a y} d y$ can be substituted, to give:

First-flight escape probability from a slab: $\quad P_{V S, 0}=\frac{1}{2 a \Sigma_{t}}\left[1-2 E_{3}\left(\Sigma_{t} a\right)\right]$

### 8.3.5.2 Escape Probability from a Sphere

In the case of a sphere of radius $a$, we always have $p(R) d R=2 \mu d \mu$. Through trigonometry, we obtain $\mu=\cos \theta=R /(2 a)$, and by differentiation, $d \mu=d R /(2 a)$, where:

$$
p(R) d R=\frac{R}{2 a^{2}} d R
$$

and $<R>=\frac{4 V}{S}=\frac{4}{3} a$
Generally, all the moments $<R^{n}>$ of a finite object exist. By using these results in Eq. 8.40, we find for the sphere (Fig. 8.18):

$$
\begin{aligned}
P_{V S, 0} & =\frac{1}{<R>\Sigma_{t}} \int_{a}^{+\infty}\left(1-e^{-\Sigma_{t} R}\right) p(R) d R \\
& =\frac{3}{4 a \Sigma_{t}} \int_{0}^{2 a} \frac{R}{2 a}\left(1-e^{-\Sigma_{t} R}\right) d R
\end{aligned}
$$

and, after integration:
First-flight escape probability from a sphere: $\quad P_{V S, 0}$

$$
\begin{equation*}
=\frac{3}{4 a \Sigma_{t}}\left(1+\frac{1}{a \Sigma_{t}} e^{-2 a \Sigma_{t}}+\frac{1}{2 a^{2} \Sigma_{t}^{2}}\left(e^{-2 a \Sigma_{t}}-1\right)\right. \tag{8.42}
\end{equation*}
$$

Fig. 8.18 Sphere of radius $a$


### 8.3.5.3 Internal Escape Probability from a Hollow Sphere

Westfall has developed ${ }^{32,33}$ the transmission probabilities for a hollow sphere assuming white or specular boundary conditions, as well as uniformly distributed isotropic sources. This corresponds to an interface current in the form of a cosine, with respect to the normal. These expressions are particularly useful for sphericalshaped fuel (pebble-bed reactor, or even micro-fuel of $H T R S$ ). Let $p_{i e}$ be the probability that a neutron leaves the internal surface isotropically, to reach the external surface without collision (the other definitions are similar in using the indices $i$ for internal, $e$ for external, and $V$ for the internal volume):

$$
p_{i e}=\frac{\int d s \int_{\vec{n} \cdot \vec{\Omega}>0} d \Omega \vec{n} \cdot \vec{\Omega} e^{-\Sigma_{t, e} \ell(\vec{\Omega})}}{\int d s \int_{\vec{n} \cdot \vec{\Omega}>0} d \Omega \vec{n} \cdot \vec{\Omega}}
$$

Owing to the spherical symmetry, this can be simplified to (Fig. 8.19):

$$
p_{i e}=\frac{\int_{y=0}^{y=r_{i}} 2 \pi y e^{-\Sigma_{l, e} \ell(y)} d y}{\int_{y=0}^{y=r_{i}} 2 \pi y d y}
$$

Setting $a=\sqrt{r_{e}^{2}-r_{i}^{2}} \Sigma_{t, e}$ and $a=\left(r_{e}-r_{i}\right) \Sigma_{t, e}$, and after some algebraic manipulations, we find:

$$
p_{i e}=\frac{1}{2 r_{i}^{2} \Sigma_{t, e}^{2}}\left[(a+1) e^{-a}-(b+1) e^{-b}+\frac{a^{4}}{b^{2}} E_{3}(b)-a^{2} E_{3}(a)\right] .
$$

By reciprocity: $p_{e i}=\left(\frac{r_{i}}{r_{e}}\right)^{2} p_{i e}$
The probability, $p_{e e}$, for a neutron arriving isotropically from the external surface to reach the external surface again without going through the internal volume $V$, can also be found:

[^161]Fig. 8.19 Hollow sphere with external radius $r_{e}$ and internal radius $r_{i}$


$$
p_{e e}=\frac{\int_{y=r_{i}}^{y=r_{e}} 2 \pi y e^{-\Sigma_{t, e} \sqrt{r_{e}^{2}-y^{2}}} d y}{\int_{y=0}^{y=r_{e}} 2 \pi y d y}=\frac{1}{2 r_{e}^{2} \Sigma_{t, e}^{2}}\left[1-(2 a+1) e^{-2 a}\right]
$$

The probability, $p_{i i}$, is given by the equation valid for any convex volume:

$$
p_{i i}=1-\langle R\rangle \Sigma_{t, i} P_{V i}=1-\frac{4}{3} r_{i} \Sigma_{t, i} P_{V i}
$$

The probability, $P_{V i}$, is related to the solid sphere problem.

### 8.3.5.4 Escape Probability from a Cylinder

The calculation for cylinder of radius $R$, mean chord length $\langle R\rangle=2 R$, is more tedious. Indeed, it involves Bessel functions (Duderstadt and Martin 1979):

$$
P_{V S, 0}=\frac{2 \Sigma_{t} R}{3}\binom{2\left[\Sigma_{t} R K_{1}\left(\Sigma_{t} R\right) I_{1}\left(\Sigma_{t} R\right)+K_{0}\left(\Sigma_{t} R\right) I_{0}\left(\Sigma_{t} R\right)-1\right]}{+K_{1}\left(\Sigma_{t} R\right) I_{0}\left(\Sigma_{t} R\right)-K_{0}\left(\Sigma_{t} R\right) I_{1}\left(\Sigma_{t} R\right)+\frac{K_{1}\left(\Sigma_{t} R\right) I_{1}\left(\Sigma_{t} R\right)}{\Sigma_{t} R}}
$$

The study of an annular cylinder, where the inner/central part is made of another material than that of the outer part, consists of calculating ${ }^{34}$ the average chord of such a cylinder (Fig. 8.20).

Let $G$ be the probability that a neutron entering isotropically through the internal surface of the cylinder does not exit the inner cylinder (sticking probability, Spanier and Gelbard $1969, \mathrm{p} 151$ ). And let $p_{i i}$ be the probability of going through the inner cylinder without collision. If we consider a neutron along the path $\vec{\Omega}$, and if $G=0$, it

[^162]Fig. 8.20 Annular cylinder with external radius $r_{e}$ and internal radius $r_{i}$

will be able to reach the right half-circumference $\pi r_{e}^{2}$ (by varying the slope of $\vec{\Omega}$ ). For a neutron along the path $\overrightarrow{\Omega_{2}}$, those on the right (half of the neutrons) of the inner cylinder will reach the external surface on the right without encountering the central cylinder while the neutrons on the left (the other half) will definitely encounter it, and will have a probability $G$ of not reaching the surface $\alpha r_{e}$. Overall, the weighted escape surface per unit height for neutrons going to the right is:

$$
\pi r_{e}^{2}-G \frac{\alpha r_{e}}{2},
$$

a quantity which will be multiplied by 2 to account for neutrons going in the opposite direction $-\vec{\Omega}$. By using $\alpha=\pi-2 \arccos \left(r_{i} / r_{e}\right)$ and $g \equiv \frac{1}{2}-\frac{\arccos \left(r_{i} / r_{e}\right)}{\pi}$, we find:

$$
\langle R\rangle=\frac{4 \pi\left(r_{e}^{2}-r_{i}^{2}\right)}{2 \pi r_{e}(1-G g)}
$$

$G$ can be calculated in terms of the probability $p_{i i}$ and the escape probability from the central cylinder $P_{V S, 0}$ where $S$ is the internal surface. Since $1-p_{i i}$ is the probability of having a collision in the internal cylinder $V$ for a neutron arriving isotropically from the internal surface, the proportion $\left(1-p_{i i}\right) \Sigma_{a, e} / \Sigma_{t, e}$ will be absorbed. From which stems the following scheme:

The quantity of neutrons absorbed is thus given by:

$$
\begin{aligned}
G & =\left(1-p_{i i}\right) \frac{\Sigma_{a, e}}{\Sigma_{t, e}}\left[1+\left(1-P_{V i, 0}\right) \frac{\Sigma_{a, e}}{\Sigma_{t, e}}+\left(1-P_{V i, 0}\right)^{2}\left(\frac{\Sigma_{s, e}}{\Sigma_{t, e}}\right)^{2}+\cdots\right] \\
& =\left(1-p_{i i}\right) \frac{\Sigma_{a, e}}{\Sigma_{t, e}} \frac{1}{1-\left(1-P_{V i, 0}\right) \frac{\Sigma_{a, e}}{\Sigma_{t, e}}}
\end{aligned}
$$

These computations allow us to take into account, for example, a partitioning of the fuel pellet to consider the rim effect of plutonium production on the surface of the fuel in spatial self-shielding.

### 8.3.5.5 Concept of Opacity

If we consider the escape probability in terms of the geometry (slab of thickness $2 R$, cylinder and sphere of radius $R$ ), a non-negligible dependence on $\Sigma_{t} R$ can be observed. In particular, the escape probability for a sphere is more important because of its compactness. On the other hand, it can be seen that in all these calculations, there arises the product of the total cross section by the mean chord, which is called opacity or blackness, often denoted by $X$ :

Opacity: $\quad X=\Sigma_{t}<R>=\frac{4 \Sigma_{t} V}{S}$
This dimensionless quantity can be regarded as the mean chord length expressed in terms of the mean free path, $1 / \Sigma_{t}$. It is shown that the first-flight escape probability $P_{V S, 0}$ shows little dependence on the shape of the medium when it is considered in terms of the opacity-which makes it an excellent parameter to characterize a medium (Fig. 8.21) (Meghreblian and Holmes 1960, p671):

It is also observed that the rational approximation of Wigner, which was seen in the chapter on resonance absorption, and which consists of approximating the firstflight escape probability by:

$$
P_{V S, 0} \approx \frac{1}{1+\Sigma_{t}\langle R\rangle}=\frac{1}{1+X}
$$

is fairly close to real life-within $20 \%$ for a $1 D$ geometry (Spanier and Gelbard 1969, p154).

### 8.3.5.6 Multiple Collision Escape Probability

If $P_{V S}$ is the first-flight escape probability (uncollided neutrons), which will be now denoted $P_{V S, 0}$ for more precision, the collision probability in the fuel for a firstflight neutron will naturally be:


Fig. 8.21 First-flight escape probability against blackness (adapted from Dresner 1960, p70)

$$
P_{V V, 1}=1-P_{V S, 0}
$$

After the collision, and assuming a uniform distribution of first collisions, the escape probability for neutrons having undergone a single collision, so far as the scattering probability is $\Sigma_{s}^{c} / \Sigma_{t}^{c}$, is therefore:

$$
P_{V S, 1}=P_{V S, 0}\left(1-P_{V S, 0} \frac{\Sigma_{s}^{c}}{\Sigma_{t}^{c}}\right.
$$

By induction, the escape probability for a neutron having undergone $n$ collisions, is:

$$
P_{V S, n}=P_{V S, 0}\left(1-P_{V S, 0}\right)^{n}\left(\frac{\Sigma_{s}^{c}}{\Sigma_{t}^{c}}\right)^{n}
$$

By summing the different contributions from successive collisions, the multiple collision escape probability is obtained as the infinite sum of a geometric ${ }^{35}$ series, since $\left(1-P_{V S, 0}\right) \Sigma_{s}^{c} / \Sigma_{t}^{c}$ is less than 1:

[^163]Multiple collision escape probability with a uniform distribution of collisions:

$$
\begin{equation*}
P_{V S}=P_{V S, 0} \sum_{n=0}^{\infty}\left(1-P_{V S, 0}\right)^{n}\left(\frac{\Sigma_{s}^{c}}{\Sigma_{t}^{c}}\right)^{n}=\frac{P_{V S, 0}}{1-\left(1-P_{V S, 0}\right) \frac{\Sigma_{s}^{c}}{\Sigma_{t}^{c}}} \tag{8.44}
\end{equation*}
$$

Using this new variable, we can write the relations linking all the relevant probabilities:

$$
\left\{\begin{array}{l}
P_{V S}=\frac{1}{X} P_{S V} \\
P_{S V}+P_{S S}=1 \\
P_{V V}+P_{V S}=1
\end{array}\right.
$$

For a strong opacity, the neutron has very little chance of crossing the volume (which explains the term opacity derived from optics). Hence, its probability of interacting in the volume when coming from the surface is $1: P_{S V} \approx 1$ and $P_{V V} \approx 1-1 / X$ which is not equal to 1 since a neutron emitted near the surface still has a chance to escape. For media with a large size when compared to the mean free path, the first-flight escape probability tends to:

$$
\lim _{V \rightarrow \infty} P_{V S}=\frac{1}{X}=\frac{S}{4 \Sigma_{t} V}
$$

Amouyal, Benoist and Horowitz have proposed, in the early 60's, corrections to take into account the spatial non-uniformity of the collision density. It will be seen in the chapter on heterogeneous reactors how to generalize this reasoning to infinity in multi-cell calculations.

### 8.3.5.7 Escape Probability in Transient States

The first-flight collision probabilities, as defined above, only have meaning in steady-state. However, we can extend the concept to transient states, by using first-flight leakage rates. The transient state transport equation with a timeindependent external source is given by:

$$
\frac{1}{v} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{g \operatorname{trad}} \Phi(\vec{r}, \vec{\Omega}, t)+\Sigma_{t} \Phi(\vec{r}, \vec{\Omega}, t)=S f(t)
$$

If a Laplace transform in time is applied to the previous equation, we obtain, with $\Phi(\vec{r}, \vec{\Omega}, p)=\mathrm{L}_{t}(\Phi)=\int_{0}^{\infty} e^{-p t} \Phi(\vec{r}, \vec{\Omega}, t) d t$ and $\Phi(\vec{r}, \vec{\Omega}, t=0)=0$ :

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, p)+\left(\Sigma_{t}+\frac{p}{v}\right) \Phi(\vec{r}, \vec{\Omega}, p)=S \mathrm{~F}(p)
$$

In the case where $f(t)=\delta(t)$, i.e., a "flash" source at $t=0$ of intensity $S$, it can be seen that $\Phi(\vec{r}, \vec{\Omega}, p)$ satisfies the usual steady-state transport equation where the term $p / v$ has been added to the total cross section. Therefore, the escape probabilities computed in steady-state can be used to obtain the value of the transient state leakage rate using the Laplace transform. For example, in the case of the slab of thickness $a$, where we had found:

$$
\begin{aligned}
P_{V S} & =\frac{1}{2 a \Sigma_{t}}\left[1-2 E_{3}\left(\Sigma_{t} a\right)\right], \text { we obtain: } \mathrm{P}_{V S}(p) \\
& =\frac{v}{2 a\left(\Sigma_{t} v+p\right)}\left[1-2 E_{3}\left(\Sigma_{t} \frac{\left(\Sigma_{t} v+p\right) a}{v}\right)\right]
\end{aligned}
$$

which, through an inverse Laplace transform, gives:

$$
P_{V S}(t)=\frac{v}{2 a} e^{-\Sigma_{t} v t}\left[\Theta(t)-\left(1-\frac{a^{2}}{v^{2} t^{2}}\right) \Theta\left(t-\frac{a}{v}\right)\right]
$$

In this equation, $\Theta(t)$ is the Heaviside (step) function. This approach works with convex geometries but Henderson and Magnard generalized ${ }^{36}$ it for solid and hollow spheres, where the inverse Laplace transform leads to very long formula but still analytical. For example, still in the case of a slab but with a source pulse of length $\Delta t$, i.e., with $f(t)=\Theta(t)-\Theta(t+\Delta t)$ :

$$
\left\{\begin{array}{l}
\kappa(t)=\left(1-e^{-\Sigma_{t} v t}\right) \Theta(t)+\left(\left(1-\frac{a^{2}}{v^{2} t^{2}}\right) e^{-\Sigma_{t} v t}-2 E_{3}\left(\Sigma_{t} a\right)+2 \frac{a^{2}}{v^{2} t^{2}} E_{3}\left(\Sigma_{t} v t\right)\right) \Theta\left(t-\frac{a}{v}\right) \\
P_{V S}(t)=\frac{1}{2 \Sigma_{t} a}[\kappa(t)-\kappa(t-\Delta t)]
\end{array}\right.
$$

[^164]Keller and Lee have generalized this approach ${ }^{37}$ by calculating the first-flight collision probability $P_{i i^{\prime} k k^{\prime}}$ depending on time, for a plane reactor, for a neutron born in the region $i$ in the time interval $k$, interacting in the region $i$ ' in the time interval $k^{\prime}$ :

$$
P_{i i^{\prime} k k^{\prime}}=\frac{\Sigma_{i k}}{\Delta_{k^{\prime}} \Delta_{i^{\prime}}} \int_{x_{i-1 / 2}}^{x_{i+1}{ }^{1 / 2}} d x \int_{x_{i^{\prime}-1 / 2}}^{x_{i^{\prime}+1 / 2}} d x^{\prime} \int_{t_{k-1 / 2}}^{t_{k+1 / 2}} d t \int_{\substack{t_{k^{\prime}-1 / 2}}}^{t_{k^{\prime}+1 / 2}} d t^{\prime} K\left(x, x^{\prime}, t, t^{\prime}\right)
$$

where $K$ is the first-flight collision operator in transient state:

$$
K\left(x, x^{\prime}, t, t^{\prime}\right)=\frac{e^{-\Sigma_{t} v\left(t-t^{\prime}\right)}}{2\left(t-t^{\prime}\right)} \Theta\left[t-t^{\prime}-\frac{\left|x-x^{\prime}\right|}{v}\right]
$$

The time-dependent flux is then given by:

$$
\Phi(x, t)=\int_{-\infty}^{+\infty} d x^{\prime} \int_{0}^{t} d t^{\prime} K\left(x, x^{\prime}, t, t^{\prime}\right) Q\left(x^{\prime}, t^{\prime}\right)
$$

### 8.3.5.8 Interface Current Method

(Stacey 2001, p315)
When the Peierls operator is integrated from an interface of the domain (assumed convex), in general, the result is such that the flux and current are non-zero at that interface. The integral form thus reveals a surface term representing the transport of neutrons at the interface in the direction $\vec{\Omega}$. Let $\overrightarrow{r_{S}}$ be a point on surface $S$, with the outwards normal denoted by $\vec{n}$, taking into account an isotropic source per unit volume, the integral form of the transport equation is given by:

$$
\Phi(\vec{r}, \vec{\Omega})=e^{-\overline{\bar{\Sigma}_{\ell}}\left(\vec{r}, \overrightarrow{r_{S}}\right)} \Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) \quad+\int_{0}^{\ell} d \ell^{\prime} \frac{e^{-\overline{\Sigma_{\ell} \ell}\left(\ell^{\prime}\right)}}{4 \pi} q\left(\vec{r}-\ell^{\prime} \vec{\Omega}\right)
$$

where $\overrightarrow{r_{S}}=\vec{r}-\ell_{S} \vec{\Omega}$ and $d^{2} \Omega=\frac{d^{2} \ell_{S} \vec{\Omega} \cdot \vec{n}}{\ell_{S}^{2}}$. Integrating over all points of the surface $S$ and the volume sources, we find (Fig. 8.22):

[^165]

Fig. 8.22 Accounting for neutron current at the boundaries

$$
\begin{aligned}
\Phi(\vec{r}) & =\int_{4 \pi} d \vec{\Omega} \Phi(\vec{r}, \vec{\Omega}) \\
& =\int_{\vec{\Omega}} \int_{\overrightarrow{r_{S}} \in S} d^{2} \Omega d \overrightarrow{r_{S}} e^{-\overline{\Sigma_{\imath} \ell}\left(\vec{r}, \overrightarrow{r_{S}}\right)} \Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) \quad+\int_{V} d \overrightarrow{r^{\prime}} \frac{\left.e^{-\overline{\Sigma_{\ell} \ell}\left(\vec{r}, \overrightarrow{r^{\prime}}\right.}\right)}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right)
\end{aligned}
$$

The surface contribution of the integrated flux is a surface integral over the incoming neutrons ( $\vec{\Omega} \cdot \vec{n}<0$ ), which is written:

$$
\int_{\vec{\Omega} . \vec{n}<0} d^{2} \ell_{S} \frac{e^{-\overline{\bar{\Sigma}_{\ell}}\left(\ell_{S}\right)}}{\ell_{S}^{2}} \vec{\Omega} \cdot \vec{n} \Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)
$$

recalling that $\vec{\Omega} \Phi\left(\overrightarrow{r_{S}}\right)$ is the neutron current and that $\vec{\Omega} \cdot \vec{n} \Phi\left(\overrightarrow{r_{S}}\right)$ is the incoming neutron flux for $\vec{\Omega} . \vec{n}<0$, and outgoing flux for $\vec{\Omega} \cdot \vec{n}>0$. Assuming that the flux at the interface is isotropic, we have:

$$
\Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)=\frac{\Phi\left(\overrightarrow{r_{S}}\right)}{4 \pi}
$$

since:

$$
\int_{\vec{\Omega} \cdot \vec{n}>0} d^{2} \Omega \vec{\Omega} \cdot \vec{n}=\int_{0}^{\pi / 2} d \theta \sin \theta \cos \theta \int_{0}^{2 \pi} d \varphi=\pi
$$

The outgoing and incoming currents, $J^{+}$and $J^{-}$are then given by:

$$
\left\{\begin{array}{l}
J^{+}=\int_{S} d^{2} r_{s} \int_{\vec{\Omega} \cdot \vec{n}>0} d^{2} \Omega \vec{\Omega} \cdot \vec{n} \Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)=\int_{S} d^{2} r_{S} \frac{\Phi\left(\overrightarrow{r_{S}}\right)}{4} \\
\left|J^{-}\right|=\int_{S} d^{2} r_{s} \int_{\vec{\Omega} \cdot \vec{n}<0} d^{2} \Omega|\vec{\Omega} \cdot \vec{n}| \Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)=\int_{S} d^{2} r_{S} \frac{\Phi\left(\overrightarrow{r_{S}}\right)}{4}
\end{array}\right.
$$

The net current $J=J^{+}-\left|J^{-}\right|$is thus indeed zero at the interface because of the isotropy of the flux, which translates to a perfect reflection condition. The interface current method ${ }^{38}$ consists in subdividing the surface of the volume $V_{i}$ into surface elements $S_{k}^{i}$ for which constant currents are assumed, such that:

$$
\sum_{k=1}^{K} S_{k}^{i}=S_{i}
$$

Each of the surfaces $S_{k}^{i}$ is also the surface of another volume $V_{j}$ in contact with $V_{i}$. The volume $V_{i}$ is itself divided into elementary volumes $V_{m}^{i}$, whose exterior surfaces will be $S_{k}^{i}$, such that:

$$
\sum_{m=1}^{M} V_{m}^{i}=V_{i}
$$

Figure 8.23 illustrates a $2 D$ example.
Since the setting of the volume $V_{i}$ is considered through the interface conditions, it is pointless to integrate the Boltzmann equation over the whole space, but rather only on the tiling of the considered volume, by introducing surface integrals induced by incoming currents:

$$
\Sigma_{m}^{i} \Phi_{m}^{i} V_{m}^{i}=\sum_{j=1}^{M} P_{j m} q_{j} V_{j}^{i}+\sum_{k=1}^{K} P_{k m} J_{k}^{i^{-}}
$$

[^166]Fig. 8.23 Tiling of a $2 D$ space


In this equation, $P_{k m}$ is the probability that a neutron entering through the surface $k$ has its first collision in the volume $V_{m}^{i}$. This probability is obtained by weighing the incoming current by the attenuation operator:

$$
P_{k m}=\frac{1}{J_{k}^{i-}} \int_{S} d^{2} r_{S} \int_{V_{m}^{i}} d \vec{r} \Sigma_{t}(\vec{r}) \frac{e^{-\overline{\Sigma_{t}}\left(\ell_{s}\right)}}{\ell_{S}^{2}} J_{k}^{i-}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) \cdot \overrightarrow{n_{k}}
$$

It will be noted that because of continuity, the current entering through the surface $S_{k}^{i}$ is equal to the outgoing current through the same surface from the adjacent volume-from which stems the coupling relations between the volumes $V_{i}$, and similarly for the fluxes. Also, there exists a relation between incoming and outgoing currents for the same macro-volume $V_{i}$. It will be pointed out that the flux at the point $\overrightarrow{r_{S}}$ is given by the contribution of the sources in the volume $V_{i}$ and one point from the opposite surface:

$$
\Phi\left(\vec{r}_{s}, \vec{\Omega}\right)=\int_{0}^{\ell_{s}} d \ell \frac{e^{-\overline{\bar{L}_{t} \ell}\left(\vec{r}_{s}-\ell \vec{\Omega}, \vec{r}_{s}\right)}}{4 \pi} q\left(\vec{r}_{S}-\ell \vec{\Omega}\right)+\Phi\left(\overrightarrow{r_{s}^{\prime}}, \vec{\Omega}\right) e^{-\overline{\bar{\Sigma}_{t} \ell\left(\overrightarrow{r_{s}}, \overrightarrow{r_{s}}\right)}}
$$

If this equation is multiplied by $\vec{\Omega} \cdot \overrightarrow{n_{k}}$, and the resulting expression is integrated over the surface $S_{k}^{i}$ for the outgoing $\left(\vec{\Omega} \cdot \overrightarrow{n_{k}}>0\right)$ contributions, we find:

$$
\begin{aligned}
\int_{S_{k}^{i}} d^{2} r_{S} \int_{\vec{\Omega} \cdot \vec{n}_{k}>0} d^{2} \Omega \vec{\Omega} \cdot \overrightarrow{n_{k}} \Phi\left(\vec{r}_{s}, \vec{\Omega}\right)= & \int_{S_{k}^{i}} d^{2} r_{S} \int_{\vec{\Omega} \cdot \overrightarrow{n_{k}}>0} d^{2} \Omega \vec{\Omega} \cdot \overrightarrow{n_{k}} \int_{0}^{\ell} d \ell \frac{\left.e^{-\overline{\varepsilon_{t} \ell}\left(\overrightarrow{r_{s}}-\ell \vec{\Omega}, \vec{r}_{s}\right.}\right)}{4 \pi} q\left(\vec{r}_{S}-\ell \vec{\Omega}\right) \\
& +\int_{S_{k}^{i}} d^{2} r_{S} \int_{\vec{\Omega} \cdot \overrightarrow{n_{k}}>0} d^{2} \Omega \vec{\Omega} \cdot \overrightarrow{n_{k}} \Phi\left(\overrightarrow{r_{s}^{\prime}}, \vec{\Omega}\right) e^{-\overline{\Sigma_{l} \ell}\left(\overrightarrow{r_{s}}, \overrightarrow{r_{s}}\right)}
\end{aligned}
$$

The first term on the right-hand side can be transformed into a volume integral over $\overrightarrow{r^{\prime}}$, while the second term can be changed to a surface integral over $\overrightarrow{r_{s}^{\prime}}$, by using the following:

$$
d \overrightarrow{r^{\prime}}=d^{3} r^{\prime}=\ell^{2} d \ell d^{2} \Omega \quad \text { and } \quad d^{2} r_{S}=\frac{\ell_{S}^{2}}{\vec{\Omega} \cdot \vec{n}} d^{2} \Omega
$$

Which can be written with the usual notations:

$$
J_{k}^{i^{+}}=\sum_{j=1}^{M} P_{j k} q_{j} V_{j}^{i}+\sum_{k^{\prime}=1}^{K} P_{k^{\prime} k} J_{k^{\prime}}^{i^{-}}
$$

where $P_{j k}$ is the probability of escaping the volume $V_{j}^{i}$ through the surface $S_{k}^{i}$, which will be calculated using the equation:

$$
P_{j k}=\frac{1}{q_{j}} \int_{S_{k}^{i}} d^{2} r_{S} \int_{V_{j}^{i}} d \vec{r} \Sigma_{t}(\vec{r}) \frac{e^{-\overline{\Sigma_{t} \ell}\left(\ell_{s}\right)}}{\ell_{S}^{2}} \vec{\Omega} \cdot \overrightarrow{n_{k}} q(\vec{r})
$$

In this way, we obtain a system of equations, which links the probabilities, but also, through current and flux continuity at the interfaces, the different macrovolumes. The albedo matrix, which couples the outgoing and incoming currents, can be full for a macro-volume but will be very sparse when considering the whole space consisting of a tiling of macro-volumes. Indeed, the number of non-zero elements increases linearly with the number of macro-volumes because of the decoupling of the regions via the currents. It will also be noted that this method is easily parallelizable, explaining the strong interest on new parallel processors.

### 8.3.6 The Integral Equation in 2D

In the case of a $2 D$ geometry, the direction $\vec{\Omega}$ will be projected in the considered plane $(O x y)$. The optical path is also projected in that plane. Instead of defining $\theta$ as the angle between the plane and the direction $\vec{\Omega}$, it will be defined as the angle between the $z$-axis and $\vec{\Omega}$. This is because it was seen in the $l D$ calculations for the escape probabilities that it was the sine of the angle between the $z$-axis and $\vec{\Omega}$ that arose and led naturally to the Bickley-Nayler function. Under these assumptions, the angular flux $\Phi(\vec{r}, \vec{\Omega})$ is given by:

$$
\Phi(\vec{r}, \vec{\Omega})=\int_{0}^{\ell} d \ell \frac{q\left(\vec{r}-\ell \vec{\Omega}_{p}\right)}{\sin \theta} e^{-\frac{\overline{\ell_{\ell} \ell}\left(\vec{r}, \vec{r}-\overrightarrow{\Omega_{p}}\right)}{\sin \theta}}+\Phi\left(\vec{r}-\ell_{S} \overrightarrow{\Omega_{p}}, \vec{\Omega}\right) e^{-\frac{\overline{\ell_{\ell} \ell}\left(\vec{r}, \vec{r}-\ell_{s} \overrightarrow{\Omega_{p}}\right)}{\sin \theta}}
$$

As usual, there is a term because of the internal sources $q$ of the volume, integrated up to the surface of the volume, and a surface term because of the boundary conditions.

### 8.3.7 Application to an Infinite Medium with a Fission Source

(Case et al. 1953; Case and Zweifel 1967)
In the case of an infinite medium with constant cross section and with only fission sources, the flux is written in the form:

$$
\Phi(\vec{r})=\int \overrightarrow{d r^{\prime}} \frac{e^{-\Sigma_{t} \mid \vec{r}-\vec{r}^{\prime}} \mid}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} q\left(\overrightarrow{r^{\prime}}\right) \quad \text { with } \quad q\left(\overrightarrow{r^{\prime}}\right)=\left(v \Sigma_{f}+\Sigma_{s}\right) \Phi\left(\overrightarrow{r^{\prime}}\right)
$$

where we will look for a solution in the spatial form (Salmon 1961; Duderstadt and Martin 1979; Tait 1964, p27):

$$
\Phi(\vec{r})=e^{\vec{B} \cdot \vec{r}}
$$

where $\vec{B}$ is an arbitrary vector of magnitude $B$. Generally, we also consider the average number of secondary neutrons defined by:

Number of secondary neutrons per collision:

$$
\begin{equation*}
c \equiv \frac{\nu \Sigma_{f}+\Sigma_{s}+2 \Sigma_{n, 2 n}+3 \Sigma_{n, 2 n}+\ldots}{\Sigma_{t}} \tag{8.45}
\end{equation*}
$$

The quantity $c \Sigma_{t}$ that cannot be split in two parts just like $v \Sigma_{f}$, is therefore the average number of secondary neutrons per mean free path (Tait 1964, p17). By substituting this spatial form of the flux in the integral equation and multiplying each term in the resulting expression by $e^{-\vec{B} \cdot \vec{r}}$, we obtain:

$$
\begin{aligned}
e^{-\vec{B} \cdot \vec{r}} e^{+\vec{B} \cdot \vec{r}} & =1 \\
& =c e^{-\vec{B} \cdot \vec{r}} \int \overrightarrow{d r^{\prime}} \Sigma_{t} \frac{e^{-\Sigma_{t} \mid \vec{r}-\vec{r}^{\prime}} \mid}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} e^{+\vec{B} \cdot \vec{r}}=c \int \overrightarrow{d r^{\prime}} \Sigma_{t} \frac{e^{-\Sigma_{t}\left[\frac{\vec{B}}{\sum_{t}} \cdot\left(\vec{r}-\overrightarrow{r^{\prime}}\right)+\left|\vec{r}-\overrightarrow{r^{\prime}}\right|\right]}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}}
\end{aligned}
$$

Fig. 8.24 Geometrical aspects of $\vec{B}$


By placing $\vec{B}$ along the $\vec{y}$ axis (Fig. 8.24), we can evaluate the previous integral, with $\ell=\left|\vec{r}-\overrightarrow{r^{\prime}}\right|, \vec{B} \cdot\left(\vec{r}-\overrightarrow{r^{\prime}}\right)=B \ell \cos \theta$ and the differential volume element, $d \overrightarrow{r^{\prime}}=\ell^{2} d \ell \sin \theta d \theta d \varphi$ :

$$
\begin{aligned}
\int \overrightarrow{d r^{\prime}} \Sigma_{t} \frac{e^{-\Sigma_{t}\left[\frac{\vec{B}}{\Sigma_{t}}\left(\vec{r}-\overrightarrow{r^{\prime}}\right)+\left|\vec{r}-\overrightarrow{r^{\prime}}\right|\right]}}{4 \pi\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} & =\frac{1}{4 \pi} \int_{0}^{2 \pi} d \varphi \int_{0}^{\pi} \sin \theta d \theta \int_{0}^{\infty} \Sigma_{t} e^{-\Sigma_{t} \ell\left(1+\frac{B}{\Sigma_{t}} \cos \theta\right)} d \ell \\
& =\frac{\Sigma_{t}}{2 B} \ln \left(\frac{1+\frac{B}{\Sigma_{t}}}{1-\frac{B}{\Sigma_{t}}}\right)
\end{aligned}
$$

This integral equation will be often encountered later, as it appears when a Fourier transform of the Boltzmann equation is done.

If $c>1$, the solution to the transcendental equation, also called dispersion, in $B / \Sigma_{t}$ (Meghreblian and Holmes 1960, p380):

Dispersion equation of Placzek: $\quad \frac{c \Sigma_{t}}{2 B} \operatorname{In}\left(\frac{1+\frac{B}{\Sigma_{t}}}{1-\frac{B}{\Sigma_{t}}}\right)=1$
is purely imaginary denoted by $i B / \Sigma_{t}$ with $B / \Sigma_{t}=\operatorname{carctg}\left(B / \Sigma_{t}\right)$.
If $c<1$, the solution is real with $B / \Sigma_{t}=c \operatorname{Argth}\left(B / \Sigma_{t}\right)$. In that case, the magnitude of $B$ physically represents an attenuation coefficient in a sub-critical medium. This is shown graphically by plotting $B$ against $c$ in Fig. 8.25.

### 8.3.8 Graphical Solution to the Dispersion Equation

Coming back to Placzek's original form, when $c>1$, we can find graphically the solutions to the equation, $\tan \frac{B}{c \Sigma_{t}}=\frac{B}{\Sigma_{t}}$ (Fig. 8.26).

Fig. 8.25 Spatial coefficient for the asymptotic flux


Fig. 8.26 Graphical solution to the dispersion equation $(c<1)$


It can be observed that there are an infinite number of positive and negative solutions, all of which are complex solutions satisfying the dispersion equation and are greater than 1 in magnitude, except for the two "central" ones. In the case where $c<1$, the graphical solution of $t h\left[B /\left(c \Sigma_{t}\right)\right]=B / \Sigma_{t}$ yields only two opposite real roots since the function $t h$ is odd (Fig. 8.27):

The dispersion equation for $c<1$ therefore has a pair of real roots $\pm B$ with a magnitude smaller than $\Sigma_{t}$ (Case and Zweifel 1967; Glasstone and Edlund 1972, p396). It will be noticed that the flux is then a linear combination of positive and negative exponentials of $i \vec{B} \cdot \vec{r}$ (for $c>1$ ) or $\vec{B} \cdot \vec{r}$ (for $c<1$ ). This flux, called asymptotic flux, therefore satisfies a general diffusion equation such as:

$$
\left\{\begin{array}{lll}
\Delta \Phi-B^{2} \Phi=0 & \text { for } & c<1 \\
\Delta \Phi+B^{2} \Phi=0 & \text { for } & c>1
\end{array}\right.
$$

Fig. 8.27 Graphical solution to the dispersion equation $(S=k \log \omega)$


In a domain without sources, $1 / B^{2}$ represents a diffusion length (Tait 1964, p28). It will later be seen how to compute an expansion of the angular part of the flux in plane geometry in the more general case of anisotropy. These calculations suggest very clearly the use of a $3 D$ Fourier transform to find a general solution to the Boltzmann equation in this geometry:

$$
\left\{\begin{array}{l}
\varphi(\vec{B})=\int \Phi(\vec{r}) e^{i \vec{B} \cdot \vec{r}} d \vec{r} \\
\Phi(\vec{r})=\frac{1}{8 \pi^{3}} \int \varphi(B) e^{-i \vec{B} \cdot \vec{r}} d \vec{B}
\end{array}\right.
$$

Substituting these expressions in the integral form of the equation, we find:

$$
\int \varphi(B) e^{-i \vec{B} \cdot \vec{r}} d \vec{B}=\int d \overrightarrow{r^{\prime}} \int d \vec{B} \frac{c \Sigma_{t}}{4 \pi} \varphi(B) e^{-i \vec{B} \cdot \vec{r}} \frac{e^{-\vec{B} \cdot\left(\overrightarrow{r^{\prime}}-\vec{r}\right)-\Sigma_{t} \mid \vec{r}-r^{\prime}} \mid}{\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}}
$$

The exponential term can be integrated to give:

$$
\int \frac{e^{-\vec{B} .\left(\overrightarrow{r^{\prime}}-\vec{r}\right)-\Sigma_{t} \mid \vec{r}-\vec{r}^{\prime}} \mid}{\left|\vec{r}-\overrightarrow{r^{\prime}}\right|^{2}} d \overrightarrow{r^{\prime}}=-i \frac{\Sigma_{t}}{2 B} \ln \left(\frac{1+i \frac{B}{\Sigma_{t}}}{1-i \frac{B}{\Sigma_{t}}}\right)=\frac{\Sigma_{t}}{B} \operatorname{Arctan} \frac{B}{\Sigma_{t}}
$$

The same transcendental equation in $B$ is obtained as in (8.46). Here again, the flux satisfies the diffusion equation seen previously. The quantity $L^{2}=1 /\left(B \Sigma_{t}\right)^{2}$ is the (asymptotic) diffusion area, the physical meaning of which will be discussed further in the chapters on diffusion.

### 8.4 Third Form of the Transport Equation: the SurfaceIntegral Form

Aside from the integro-differential and integral forms, there exists a third form of the Boltzmann equation, less known, which has been explored largely by Pierre Benoist and Alain Kavenoky ${ }^{39}$ at the end of the 60 's, then in the 70 's. ${ }^{40,41}$
${ }^{39}$ Alain Kavenoky (1939-). After his studies at Ecole Polytechnique in Paris (matriculated in 1960), and then at the Ecole des Ponts et Chaussées (1965), he joins the CEA where he successfully completes his thesis on the transport equation in 1973. His contribution at CEA/SERMA to the APOLLO1 code development is substantial.

(the Marguet collection)
${ }^{40}$ Pierre Benoist, Alain Kavenoky: A new method of approximation of the Boltzmann equation, Nuclear Science and Engineering, 32, p225 (1968). Alain Kavenoky (1939-) was the student of Pierre Benoist after his studies at the Ecole Polytechnique (1962), and his DEA (Diplôme d'Etudes Appronfondies - Diploma of Profound Studies) in 1965. His state doctoral thesis (La méthode $C_{n}$ de résolution de l'équation du transport [The $C_{n}$ method for solving the transport equation], 1973) finds its place in the long-standing French tradition of neutronics, with Jacques Yvon as president, and Jules Horowitz, Jean Bussac and Pierre Benoist as jury members. It will impact significantly the 70's. The $C_{n}$ method that is developed in it, led to the publication of about ten conference and prestigious journal papers. Kavenoky was thereafter head of the Physics and Mathematics group of the CEA/SERMA in Saclay, and contributed substantially to the development of APOLLO1. After that, he was a member of the Scientific, Pedagogical and Technological Mission of the CNRS, tasked with intensive computations, and took care of funding for various university projects.

The Marguet collection


[^167]This surface-integral form, which would be aptly called the BenoistKavenoky form since it had not been really used before their innovative works, is based on a complementary property of the Boltzmann equation, called Placzek's lemma.

### 8.4.1 Placzek's Lemma



George Placzek (Public domain)
Consider a sub-critical medium, at the limit of being critical (but not super-critical such that there can exist a steady-state solution), surrounded by its outer surface $S$. This medium, characterized by a number $c$ of secondary neutrons is finite (of volume $V$ ) and surrounded by vacuum. It is shown that this problem is rigorously equivalent to the infinite case where the medium fills the whole space, but where the sources are removed outside of $V$, while those inside are kept, and where a surface source is added to $S$ with an intensity $-\vec{\Omega} \cdot \vec{n} \Phi_{\text {finite }}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$, with $\vec{n}$ being the outside normal to a point $\overrightarrow{r_{S}}$ of the surface $S$, and $\Phi_{\text {finite }}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ is the angular flux of the (first) finite problem (Fig. 8.28).

[^168]

Fig. 8.28 Placzek's lemma

In the case of a super-critical problem, the solution of the infinite problem is chosen such that the angular flux is zero outside of $V$. This lemma is proven by considering the angular flux $\Theta(\vec{r}, V) \Phi_{\text {finite }}(\vec{r}, \vec{\Omega})$, differentiated from the solution of the flux to the finite problem. $\Theta(\vec{r}, V)$ is the volume Heaviside function, which is 1 in the volume $V$ and zero elsewhere. Since the Boltzmann equation is the same in the volume for the two cases, $\Phi_{\infty}(\vec{r}, \vec{\Omega}) \equiv \Theta(\vec{r}, V) \Phi_{\text {finite }}(\vec{r}, \vec{\Omega})$ is of course the solution to the infinite case since $\Theta(\vec{r}, V) \equiv 1$ in the volume. The added surface source creates an angular flux discontinuity at the interface such that:

$$
\Phi_{\infty}\left({\overrightarrow{r_{S}}}^{-}, \vec{\Omega}\right)=\Phi_{\infty}\left({\overrightarrow{r_{S}}}^{+}, \vec{\Omega}\right)-\Phi_{\text {finite }}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)
$$

In these, $\overrightarrow{r S}^{-}=\lim _{\varepsilon \rightarrow 0}\left(\overrightarrow{r_{S}}-\varepsilon \vec{n}\right)$ and ${\overrightarrow{r_{S}}}^{+}=\lim _{\varepsilon \rightarrow 0}\left(\overrightarrow{r_{S}}+\varepsilon \vec{n}\right)$. The function $\Theta(\vec{r}, V)$ $\Phi_{\text {finite }}(\vec{r}, \vec{\Omega})$ satisfies this equation by construction. At the interface $S$, the outgoing angular current from the finite problem is $\vec{\Omega} . \vec{n} \Phi_{\text {finite }}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$. If a source removing a current $-\vec{\Omega} . \vec{n} \Phi_{\text {finite }}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ is added, the result of these two components, because of the linearity of the Boltzmann equation for external sources in a purely scattering medium, is a null current at the surface $S$ of the infinite problem for outgoing ( $\vec{\Omega} . \vec{n} \geq 0$ ) directions of the volume $V$ (and hence, incoming directions for the complementary infinite medium). Since there are no sources external to $V$ in the infinite case, the flux is naturally zero (by construction). It is in fact the point of this clever construction regarding the infinite medium. In this case, the flux $\Theta(\vec{r}, V) \Phi_{\text {finite }}$ $(\vec{r}, \vec{\Omega})$ is also zero outside the volume because of the Heaviside function. And hence,
this proves Placzek's lemma. The lemma is easily generalized in multi-group by considering a source depending on energy, while taking into account the slowingdown source.

### 8.4.2 Flux Equation at the Interface

According to Placzek's lemma, we can express the Boltzmann equation as an integral equation in terms of the flux at the interface $S$, and not that in the volume anymore. This flux will be obtained by applying a Green's function $G\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}, \vec{r}, \vec{\Omega}\right)$, in infinite medium, easily calculated by a Fourier transform using methods already discussed. Consider a volume source $S(\vec{r}, \vec{\Omega})$ inside the medium and a superficial "incoming" source, which emits towards the inside, i.e., $\Phi^{+}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ for $\vec{\Omega} . \vec{n} \leq 0$ and an "outgoing" source $\Phi^{-}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ for $\vec{\Omega} . \vec{n} \geq 0$. The angular flux at any point is given by:

$$
\begin{align*}
\Phi(\vec{r}, \vec{\Omega})= & \int_{V} S\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) G\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}, \vec{r}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{3} r^{\prime} \\
& -\int_{S} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{n} \leq 0} \overrightarrow{\Omega^{\prime}} \cdot \vec{n} \Phi^{+}\left(\overrightarrow{r_{S^{\prime}}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S^{\prime}}}, \overrightarrow{\Omega^{\prime}}, \vec{r}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r^{\prime} \\
& -\int_{S} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{n} \geq 0} \cdot \vec{n} \Phi^{-}\left(\overrightarrow{r_{S^{\prime}}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S^{\prime}}}, \overrightarrow{\Omega^{\prime}}, \vec{r}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r \tag{8.47}
\end{align*}
$$

If $\vec{r}$ tends towards a surface point $\overrightarrow{r_{S}}$, we find:

$$
\begin{aligned}
\Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)= & \int_{V} S\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) G\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{3} r^{\prime} \\
& -\int_{S} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{n} \leq 0} \overrightarrow{\Omega^{\prime}} \cdot \vec{n} \Phi^{+}\left(\overrightarrow{r_{S^{\prime}}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S^{\prime}}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r^{\prime} \\
& -\int_{S} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{n} \geq 0} \overrightarrow{\Omega^{\prime}} \cdot \vec{n} \Phi^{-}\left(\overrightarrow{r_{S^{\prime}}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S^{\prime}}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r
\end{aligned}
$$

This equation links all the points on the surface. Assuming that the incoming flux $\Phi^{+}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ for $\vec{\Omega} . \vec{n} \leq 0$ is known, the third form of the Boltzmann equation can be written:

$$
\left\{\begin{aligned}
\Phi^{+}\left(\overrightarrow{r_{s}}, \vec{\Omega}\right) & =\int_{V} S\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}\right) G\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{3} r^{\prime} \\
& -\int_{S}^{V} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{\cdot} \leq 0} \overrightarrow{\Omega^{\prime}} \cdot \vec{n} \Phi^{+}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r^{\prime} \\
& -\int_{S} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{n} \geq 0}^{\Omega^{\prime}} \cdot \vec{n} \Phi^{-}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r \\
\Phi^{-}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) & =\int_{V}^{V} S\left(\vec{r}^{\prime}, \overrightarrow{\Omega^{\prime}}\right) G\left(\overrightarrow{r^{\prime}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{3} r^{\prime} \\
& -\int_{S} \int_{\overrightarrow{\Omega^{\prime}} \cdot \vec{n} \leq 0} \overrightarrow{\Omega^{\prime}} \cdot \vec{n} \Phi^{+}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r^{\prime} \\
& -\int_{S} \int_{\vec{\Omega}^{\prime} \cdot \vec{n} \geq 0} \overrightarrow{\Omega^{\prime}} \cdot \vec{n} \Phi^{-}\left(\overrightarrow{r_{S}}, \vec{\Omega}\right) G\left(\overrightarrow{r_{S}}, \overrightarrow{\Omega^{\prime}}, \overrightarrow{r_{S}}, \vec{\Omega}\right) d \overrightarrow{\Omega^{\prime}} d^{2} r
\end{aligned}\right.
$$

Once the angular fluxes at the surface are known, the flux at any point can be obtained using Eq. 8.47.

### 8.4.3 Application to the Milne Problem

Consider a plane geometry. The Milne problem, which will be further discussed in Chap. 9, consists of studying the outgoing angular flux from a semi-infinite plane submitted to an exterior radiation (astrophysics problem). The problem, where an incoming angular flux is imposed, is written using the cosine of the deviation angle (with respect to the positive $x$ axis), when hitting the plane:

$$
\Phi^{+}(\mu)=\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) d \mu^{\prime}+\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \text { for } \mu>0
$$

This equation links the outgoing flux $\Phi^{-}$at the interface to the incoming flux. The Green's function is decomposed into an uncollided flux (denoted $G_{\text {unc }}$ ) and a multiple-collision flux (denoted $G_{m c}$ ):

$$
G\left(\mu^{\prime}, \mu\right)=G_{u n c}\left(\mu^{\prime}, \mu\right)+G_{m c}\left(\mu^{\prime}, \mu\right)=\frac{1}{\mu}\left(\mu-\mu^{\prime}\right)+G_{m c}\left(\mu^{\prime}, \mu\right)
$$

By substituting this form of the Green's function into the flux equation, we have,

$$
\left\{\begin{array}{l}
0=\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}+\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \text { for } \mu>0 \\
\Phi^{+}(\mu)=\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}+\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \text { for } \mu<0
\end{array}\right.
$$

### 8.4.4 Second Complementarity Theorem

The linearity of the integro-differential equation is used to define the solution of the problem with a heterogeneous medium, finite or infinite, as the combination of two "overlapped" problems. Inside the medium, a convex surface $S$ is designated, such that it surrounds a volume $V$, with the flux at the interface being $\Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$. Using a similar line of reasoning as Placzek's lemma, the flux at any point can be reconstructed by computing a second problem where this volume $V$ is mentally placed inside an infinite black body. The sources inside $V$ are retained but a source of strength $\Theta(-\vec{\Omega} \cdot \vec{n}) \Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ is imposed at the surface $S$ only for incoming directions $(\vec{\Omega} \cdot \vec{n}<0)$ with $\Theta$ as the Heaviside function. To this second problem, the solution of a third problem is added. This latter problem is obtained by, this time, substituting the volume $V$ by a black body and imposing a surface source $\Theta(\vec{\Omega} \cdot \vec{n})$ $\Phi\left(\overrightarrow{r_{S}}, \vec{\Omega}\right)$ at $S$ for outgoing directions $\vec{\Omega} \cdot \vec{n}>0$,

$$
\Phi(\vec{r}, \vec{\Omega})=\Phi_{2}(\vec{r}, \vec{\Omega})+\Phi_{3}(\vec{r}, \vec{\Omega})
$$

The second problem is rigorously identical to that investigated during the proof of Placzek's lemma. The same goes for the third problem, to the extent that the fact the volume is a black body amounts to making the surface $S$ convex with respect to the outside (no neutron will be able to cross $V$ to appear on the other side) (Fig. 8.29).

The third form of the Boltzmann equation has the advantage of using only the angular fluxes at the interfaces: the amount of calculations required for resolution is therefore not dependent on the size of the media-which can be aptly used during the meshing of the studied problem.


Fig. 8.29 Second complementarity theorem

### 8.5 Concept of Characteristic Function

In an infinite homogeneous and isotropic medium, there exists a Green's operator $G\left(\vec{r}-\overrightarrow{r^{\prime}}\right)$ which relates a point source $S\left(\overrightarrow{r^{\prime}}\right)$ to a flux $\Phi(\vec{r})$ by the convolution equation:

$$
\Phi(\vec{r})=G\left(\vec{r}-\overrightarrow{r^{\prime}}\right)\left\lfloor S\left(\overrightarrow{r^{\prime}}\right)\right\rfloor
$$

Let $\varphi(B), g(B)$ and $s(B)$ be the respective Fourier transforms of the previous functions. The Fourier transform of a convolution being the product of the Fourier transforms, ${ }^{42}$ we can write:

$$
\varphi(B)=g(B) s(B)
$$

[^169]Since the medium is isotropic, $G\left(\vec{r}-\overrightarrow{r^{\prime}}\right)$ depends only on the norm of its argument, and so does $g(B)$. The characteristic function is then defined as the inverse Fourier transform of $G\left(\vec{r}-\overrightarrow{r^{\prime}}\right)$ :

Characteristic function: $\quad \psi(B)=\frac{1}{g(B)}$
The characteristic function is closely tied to the theory used to describe the movement of neutrons. Hence, in diffusion theory, the flux from a point source $\delta(\vec{r})$ is given by the Green's function in spherical coordinates:

$$
\Phi(r)=\frac{1}{4 \pi D r} e^{-\frac{r}{L}}=G(r)
$$

where the Fourier transform in $3 D^{43}$ is written:

$$
g(B)=\int_{4 \pi} G(r) e^{i \vec{B} \cdot \vec{r}} d^{3} r=\int_{0}^{+\infty}\left(\frac{1}{4 \pi D r} e^{-\frac{r}{L}}\right) \frac{\sin B r}{B r} 4 \pi r^{2} d r=\int_{0}^{+\infty} \frac{1}{D B} e^{-\frac{r}{L}} \sin B r d r
$$

This integral is evaluated by noticing that $\sin B r$ is the imaginary part of $e^{i B r}$ :

$$
\int_{0}^{+\infty} \frac{1}{D B} e^{-\frac{r}{L}} e^{i B r} d r=\frac{1}{D B}\left[\frac{e^{\left(i B-\frac{1}{L}\right) r}}{i B-\frac{1}{L}}\right]_{0}^{+\infty}=\frac{1}{D B}\left(\frac{1}{\frac{1}{L}-i B}\right)=\frac{L}{D B\left(1+L^{2} B^{2}\right)}+i \frac{L^{2}}{D\left(1+L^{2} B^{2}\right)}
$$

where
Characteristic function for diffusion: $\quad g(B)$

$$
\begin{equation*}
=\frac{L^{2}}{D\left(1+L^{2} B^{2}\right)}=\frac{1}{\Sigma_{A}\left(1+L^{2} B^{2}\right)} \quad \text { and } \quad \psi(B)=\Sigma_{A}\left(1+L^{2} B^{2}\right) \tag{8.49}
\end{equation*}
$$

The function $g(B)$ can be expanded in terms of a power series in $B$ by expanding:

$$
\sin B r=B r-\frac{(B r)^{3}}{3!}+\frac{(B r)^{5}}{5!}-\frac{(B r)^{7}}{7!}+\ldots
$$

[^170]to give:
\[

$$
\begin{aligned}
g(B) & =\int_{0}^{+\infty} G(r) \frac{\sin B r}{B r} 4 \pi r^{2} d r \\
& =\int_{0}^{+\infty} G(r) 4 \pi r^{2} d r-\frac{B^{2}}{3!} \int_{0}^{+\infty} r^{2} G(r) 4 \pi r^{2} d r+\frac{B^{4}}{5!} \int_{0}^{+\infty} r^{4} G(r) 4 \pi r^{2} d r-\ldots
\end{aligned}
$$
\]

If the function $G(r)$ is made dimensionless, it is sufficient to relate the source (in $\left[\mathrm{n} / \mathrm{cm}^{3} / \mathrm{s}\right]$ ) to a reaction rate with the same units, for example, the absorption rate:

$$
\Sigma_{a} \Phi(\vec{r})=G\left(\vec{r}-\overrightarrow{r^{\prime}}\right)\left\lfloor S\left(\overrightarrow{r^{\prime}}\right)\right]
$$

The characteristic function is modified accordingly:

$$
g(B)=\frac{1}{1+L^{2} B^{2}} \quad \text { and } \quad \psi(B)=1+L^{2} B^{2}
$$

This normalization is interesting in so far as:

$$
\int_{0}^{+\infty} G(r) 4 \pi r^{2} d r=\int_{0}^{+\infty} \frac{1}{4 \pi L^{2}} \frac{e^{-\frac{r}{L}}}{r} 4 \pi r^{2} d r=\Gamma(2)=1
$$

The transform of $G$ can then be calculated more precisely:

$$
g(B)=1-\frac{B^{2}}{3!}\left\langle r^{2}\right\rangle+\frac{B^{2}}{5!}\left\langle r^{4}\right\rangle-\frac{B^{4}}{7!}\left\langle r^{6}\right\rangle \ldots
$$

where $\left\langle r^{n}\right\rangle$ is the average of the "crow flight" distance travelled by the neutron raised to the $n$-th power. For the diffusion operator:

$$
\int_{0}^{+\infty} r^{2} G(r) 4 \pi r^{2} d r=\int_{0}^{+\infty} r^{2} \frac{1}{4 \pi L^{2}} \frac{e^{-\frac{r}{L}}}{r} 4 \pi r^{2} d r=L^{n} \Gamma(n+2)=L^{n}(n+1)!
$$

Hence, in diffusion: $g(B)=1-L^{2} B^{2}+L^{4} B^{4}-L^{6} B^{6} \ldots=\frac{1}{1+L^{2} B^{2}}$
The already-obtained expression for $g(B)$ is found again through a limited expansion. We also recover the fact that in diffusion theory, $\left\langle r^{2}\right\rangle=6 L^{2}$, by
identifying the coefficient of $B^{2}$. When applied to monoenergetic transport equation with scattering and isotropic source, it is seen that:

$$
\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t} \Phi(\vec{r}, \vec{\Omega})=\underbrace{\int_{0}^{\infty} d E \int_{0}^{\infty} d E^{\prime} \int_{\overrightarrow{\Omega^{\prime}}} d \vec{\Omega}^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \overrightarrow{\Omega^{\prime}}\right)}_{\frac{1}{4 \pi} \Sigma_{s} \int_{\Lambda_{\pi}} \Phi\left(\vec{r}, \overrightarrow{\Omega^{\prime}}\right) d \overrightarrow{\Omega^{\prime}}}+\frac{S(\vec{r})}{4 \pi}
$$

The associated characteristic function can be found by replacing $\Phi(\vec{r}, \vec{\Omega})$ by $\phi(\vec{\Omega}) e^{i \vec{B} \cdot \vec{r}}$, and the source by $\psi(B) e^{i \vec{B} \cdot \vec{r}}$. This approach is identical to taking the Fourier transform of the equation. By construction:

$$
\int_{4 \pi} \phi(\vec{\Omega}) d \vec{\Omega}=1
$$

By substituting in the equation, we find:

$$
i \vec{\Omega} \cdot \vec{B} \phi(\vec{\Omega}) e^{i \vec{B} \cdot \vec{r}}+\Sigma_{t} \phi(\vec{\Omega}) e^{i \vec{B} \cdot \vec{r}}=\frac{1}{4 \pi} \Sigma_{s} e^{i \vec{B} \cdot \vec{r}}+\frac{\psi(B) e^{i \vec{B} \cdot \vec{r}}}{4 \pi}
$$

where: $\phi(\vec{\Omega})=\frac{1}{4 \pi\left(\Sigma_{t}+i \vec{\Omega} \cdot \vec{B}\right)}\left(\Sigma_{s}+\psi(B)\right)$.
The function $\psi(B)$ is obtained by integrating over $\vec{\Omega}$, to give:

$$
\int_{4 \pi} \phi(\vec{\Omega}) d \vec{\Omega}=1=\frac{1}{4 \pi}\left(\Sigma_{s}+\psi(B)\right) \int_{4 \pi} \frac{1}{\left(\Sigma_{t}+i \vec{\Omega} \cdot \vec{B}\right)} d \vec{\Omega}=\frac{1}{4 \pi}\left(\Sigma_{s}+\psi(B)\right) \int_{-1}^{1} 2 \pi \frac{1}{\left(\Sigma_{t}+i \mu B\right)} d \mu
$$

where $\mu$ is the cosine of the angle between $\vec{B}$ and $\vec{\Omega}$, and $d \vec{\Omega}=2 \pi d \mu$. Also:

$$
\int_{-1}^{1} \frac{1}{\left(\Sigma_{t}+i \mu B\right)} d \mu=\frac{1}{\Sigma_{t}} \int_{0}^{1} \frac{1}{\left(1+i \mu \frac{B}{\Sigma_{t}}\right)}+\frac{1}{\left(1-i \mu \frac{B}{\Sigma_{t}}\right)} d \mu=\frac{1}{i B}\left[\ln \frac{\left(1+i \mu \frac{B}{\Sigma_{t}}\right)}{\left(1-i \mu \frac{B}{\Sigma_{t}}\right)}\right]_{0}^{1}=\frac{2}{B}\left[\operatorname{Arctan}\left(\mu \frac{B}{\Sigma_{t}}\right)\right]_{0}^{1}
$$

such that, finally:
Characteristic function in homogeneous isotropic transport:

$$
\begin{equation*}
\psi(B)=\frac{B}{\operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)}-\Sigma_{s} \tag{8.50}
\end{equation*}
$$

For a function, $G(\vec{r})$ normalized such that $\Sigma_{a} \Phi(\vec{r})=G\left(\vec{r}-\overrightarrow{r^{\prime}}\right)\left\lfloor S\left(\vec{r}^{\prime}\right)\right\rfloor$, the characteristic function is written as follows:

$$
\psi(B)=\frac{B}{\Sigma_{a} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)}-\frac{\Sigma_{s}}{\Sigma_{a}}
$$

### 8.6 Fourier Transform of the Boltzmann Equation

### 8.6.1 Formalism

Let us start again with the classic Boltzmann equation with an angular source:
$\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t} \Phi(\vec{r}, \vec{\Omega})=\int_{0}^{\infty} d E \int_{0}^{\infty} d E^{\prime} \int_{\vec{\Omega}^{\prime}} d \vec{\Omega}^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, E^{\prime}, \overrightarrow{\Omega^{\prime}}\right)+S(\vec{r}, E, \vec{\Omega})$
The Fourier transform of the flux applied to an infinite and homogeneous medium is written:

$$
\varphi(E, \vec{B}, \vec{\Omega}) \equiv \int_{\vec{r}} e^{-i \vec{B} \cdot \vec{r}} \Phi(\vec{r}, E, \vec{\Omega}) d \vec{r}
$$

Usually, an arbitrary vector $\vec{k}$ is used in the exponential, but it will later be seen, that in this case, this vector has the meaning of a Laplacian, hence the more suitable notation of $\vec{B}$. The inverse Fourier transform yields the flux:

$$
\Phi(\vec{r}, E, \vec{\Omega})=\frac{1}{8 \pi^{3}} \int_{\vec{B}} e^{+i \vec{B} \cdot \vec{r}} \varphi(E, \vec{B}, \vec{\Omega}) d \vec{B}
$$

The Fourier transform of the Boltzmann equation is written:

$$
\left(i \vec{B} \cdot \vec{r}+\Sigma_{t}\right) \varphi(E, \vec{B}, \vec{\Omega})=\int_{4 \pi} d \vec{\Omega}^{\prime} \int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right) \varphi\left(E^{\prime}, \vec{B}, \overrightarrow{\Omega^{\prime}}\right)+s(E, \vec{B}, \vec{\Omega})
$$

With: $s(E, \vec{B}, \vec{\Omega}) \equiv \int_{\vec{r}} e^{-i \vec{B} \cdot \vec{r}} S(\vec{r}, E, \vec{\Omega}) d \vec{r}$.
By using the integration over angle, $\varphi(E, \vec{B}) \equiv \int_{4 \pi} \varphi(E, \vec{B}, \vec{\Omega}) d \vec{\Omega}$ (it should be pointed out that the symbol for the variable $\varphi$ is unchanged to simplify notation, hence the importance of the dependencies), and the Boltzmann equation can be integrated over angle:

$$
\varphi(E, \vec{B})=\int_{4 \pi} \frac{1}{\left(i \vec{B} \cdot \vec{r}+\Sigma_{t}\right)} d \vec{\Omega}\left(\int_{0}^{\infty} d E^{\prime} \frac{\Sigma_{s}\left(E^{\prime} \rightarrow E\right)}{4 \pi} \varphi\left(E^{\prime}, \vec{B}\right)\right)+s(E, \vec{B})
$$

With $s(E, \vec{B}) \equiv \int_{4 \pi} s(E, \vec{B}, \vec{\Omega}) d \vec{\Omega}$ and an isotropic scattering cross section:

$$
\Sigma_{s}\left(E^{\prime} \rightarrow E, \overrightarrow{\Omega^{\prime}} \rightarrow \vec{\Omega}\right)=\frac{\Sigma_{s}\left(E^{\prime} \rightarrow E\right)}{4 \pi}
$$

By placing the vector $\vec{B}=\overrightarrow{B r}$ along the polar axis and using $\mu=\cos \theta \equiv \cos \vec{\Omega} \cdot \vec{r}$, we obtain:

$$
\begin{aligned}
\int_{4 \pi} \frac{1}{4 \pi\left(i \vec{B} \cdot \vec{r}+\Sigma_{t}\right)} d \vec{\Omega} & =\int_{0}^{2 \pi} d \varphi \int_{-\pi}^{+\pi} d \theta \frac{\sin \theta d \theta d \varphi}{4 \pi\left(i B \cos \theta+\Sigma_{t}\right)} \\
& =\int_{-1}^{+1} \frac{d \mu}{2\left(i B \mu+\Sigma_{t}\right)}=\frac{1}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)=\frac{1}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)
\end{aligned}
$$

if we set:

$$
\Sigma_{t}(B) \equiv \frac{B}{\operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)} .
$$

If this expression is expanded in a power series of $B$, it is found:

$$
\Sigma_{t}(B) \approx \Sigma_{t}+\frac{1}{3 \Sigma_{t}} B^{2}+O\left(B^{4}\right)
$$

The Fourier-transformed and angularly-integrated Boltzmann equation can be written:

Fourier transform of the Boltzmann equation:

$$
\begin{equation*}
\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \varphi\left(E^{\prime}, \vec{B}\right)-\Sigma_{t}(B) \varphi(E, \vec{B})+s(E, \vec{B})=0 \tag{8.51}
\end{equation*}
$$

It should be noted that this equation coincides with Boltzmann equation for the real flux in the particular case where the flux is spatially uniform (no gradient terms) and where $\Sigma_{t}(B)$ is replaced by the usual cross section, $\Sigma_{t}$, depending on energy. Also note that $\Sigma_{t}(B=0)=\Sigma_{t}$. Thus, the equation corresponds to that for a spatially uniform flux, which confirms the Laplacian equivalence of $B$. It is also interesting to observe that the use of the expansion of $\Sigma_{t}(B)$ limited to the $B^{2}$ term in the previous equation allows us to recover the diffusion equation.

In the general case, the medium is not homogeneous and the sources, as well as scattering, are not isotropic. If an expansion in spherical harmonics is done for the flux, the same Eq. 8.51 is obtained, without assuming an isotropic medium, but retaining only the isotropic part of flux. This is the $B_{0}$ approximation.

### 8.6.2 Resolution Using Green's Function

Works on the modelling of the Boltzmann equation using Green's function (for example in slab geometry for monokinetic neutrons ${ }^{44}$ ) appeared in USA at the beginning of the 1960s. Recall that the Green's function of the transport problem corresponds to the flux created by a unit source $\delta^{3}\left(\vec{r}-\overrightarrow{r_{0}}\right) \delta\left(E-E_{0}\right)$ placed at energy $E_{0}$ and at point $\overrightarrow{r_{0}}$ in space. Subject to knowing how to calculate all the possible Green's functions, the flux from an arbitrary source is then easily calculated by integration over space and energy:

$$
\Phi(E, \vec{r})=\int_{E_{0}=0}^{E_{0}=\infty} d E_{0} \int_{\overrightarrow{r_{0}}} G\left(\vec{r}, \overrightarrow{r_{0}} E, E_{0}\right) S\left(E_{0}, \overrightarrow{r_{0}}\right) d \overrightarrow{r_{0}}
$$

Also recall that in Cartesian geometry:
$\overrightarrow{d r} \equiv d x d y d z \quad$ and $\quad \delta\left(z-z_{0}\right)=\int_{x_{0}=-\infty}^{x_{0}=+\infty} d x_{0} \int_{y_{0}=-\infty}^{y_{0}=+\infty} d y_{0} \delta^{3}\left(\vec{r}-\overrightarrow{r_{0}}\right)$, in cylindrical geometry:
$\overrightarrow{d r} \equiv r d r d \theta d z \quad$ and $\quad \delta^{3}\left(\vec{r}-\overrightarrow{r_{0}}\right)=\frac{1}{r_{0}} \delta\left(r-r_{0}\right) \delta\left(\theta-\theta_{0}\right) \delta\left(z-z_{0}\right)$,
in spherical geometry:

$$
\overrightarrow{d r} \equiv r^{2} d r d \Omega \quad \text { and } \quad \delta^{3}\left(\vec{r}-\overrightarrow{r_{0}}\right)=\frac{1}{r_{0}^{2}} \delta\left(r-r_{0}\right) \delta\left(\vec{\Omega}-\overrightarrow{\Omega_{0}}\right)
$$

The Fourier transform of the Green's function $g\left(E, E_{0}, \vec{B}, \overrightarrow{r_{0}}\right) \equiv$ $\int_{\vec{r}} e^{-i \vec{B} \cdot \vec{r}} G\left(\vec{r}, \overrightarrow{r_{0}}, E, E_{0}\right) d \vec{r}$ satisfies the equation:

$$
\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) g\left(E^{\prime}, E_{0}, \vec{B}, \overrightarrow{r_{0}}\right)-\Sigma_{t}(B) g\left(E, E_{0}, \vec{B}, \overrightarrow{r_{0}}\right)+e^{-i \vec{B} \cdot \overrightarrow{r_{0}}} \delta\left(E-E_{0}\right)=0
$$

Assuming that the solution $\phi\left(E, E_{0},\|\vec{B}\|\right)$ to the integral equation is unique:
Slowing-down/thermalization equation for a point source in energy:

$$
\begin{equation*}
\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(E^{\prime}, E_{0},\|\vec{B}\|\right)-\Sigma_{t}(B) \phi\left(E, E_{0},\|\vec{B}\|\right)+\delta\left(E-E_{0}\right)=0 \tag{8.52}
\end{equation*}
$$

The Fourier transform of the Green's function can then be calculated as:

$$
g\left(E, E_{0}, \vec{B}, \overrightarrow{r_{0}}\right)=e^{-i \vec{B} \cdot \overrightarrow{r_{0}}} \phi\left(E, E_{0},\|\vec{B}\|\right)
$$

[^171]which translates to a separation of variables (of space and energy) for some welldetermined values of $B \equiv\|\vec{B}\|$. The inverse Fourier transform yields the original Green's function:
$$
G\left(\vec{r}, \overrightarrow{r_{0}}, E, E_{0}\right)=\frac{1}{8 \pi^{3}} \int_{\vec{B}} e^{+i \vec{B} \cdot\left(\vec{r}-\overrightarrow{r_{0}}\right)} \phi\left(E, E_{0}, B\right) \overrightarrow{d B}
$$

In Cartesian geometry, we obtain:

$$
G\left(z, z_{0} E, E_{0}\right)=\frac{1}{2 \pi} \int_{B=-\infty}^{B=+\infty} e^{+i B \cdot\left(Z-Z_{0}\right)} \phi\left(E, E_{0}, B\right) d B
$$

In an infinite and homogeneous medium, the fact that the Green's function depends only on the distance $\left\|\vec{r}-\overrightarrow{r_{0}}\right\|$ is seen again.

José Guasp ${ }^{45}$ is credited with having analyzed in 1970 the mathematical behavior of the solutions $\phi\left(E, E_{0}, B\right)$ of Eq. 8.52 for thermalization theory. For that, a particular form of the scattering cross section $\Sigma_{s}\left(E^{\prime} \rightarrow E\right)$ has to be chosen, and he went with Cadilhac "secondary model", which features interesting semifactorization properties but is limited to being able to be applied only to monocrystalline media (showing a Bragg cutoff). The secondary model allows us to simplify Eq. 8.52 into a second-order differential equation involving functions specific to a considered moderator. The analysis of Eq. 8.52 suggests the decomposition of its solution $\phi\left(E, E_{0}, B\right)$ into a regular part and a singular part in energy:

[^172]
(Courtesy Guasp)
$$
\phi\left(E, E_{0}, B\right)=\bar{\phi}\left(E, E_{0}, B\right)+A\left(E_{0}, B\right) \delta\left(E-E_{0}\right)
$$

By substituting this decomposition in Eq. 8.52, it is easily found that:

$$
A\left(E_{0}, B\right)=\frac{1}{\Sigma_{t}\left(E_{0}, B\right)}
$$

It is therefore the last term, which carries the monoenergetic contribution of the neutrons not having undergone any collisions yet. The Green's function hence consists of two terms:

$$
\begin{aligned}
G\left(\vec{r}, \overrightarrow{r_{0}}, E, E_{0}\right) & =\frac{1}{8 \pi^{3}} \int_{\vec{B}} e^{+i \vec{B} \cdot\left(\vec{r}-\overrightarrow{r_{0}}\right)} \phi\left(E, E_{0}, B\right) d \vec{B}= \\
& =\frac{1}{8 \pi^{3}} \int_{\vec{B}} e^{+i \vec{B} \cdot\left(\vec{r}-\overrightarrow{r_{0}}\right)} \bar{\phi}\left(E, E_{0}, B\right) d \vec{B}+\frac{1}{8 \pi^{3}} \int_{\vec{B}} e^{+i \vec{B} \cdot\left(\vec{r}-\overrightarrow{r_{0}}\right)} \frac{\delta\left(E-E_{0}\right)}{\Sigma_{t}\left(E_{0}, B\right)} d \vec{B}
\end{aligned}
$$

In Cartesian geometry, the singular part is written:

$$
\begin{aligned}
\frac{1}{2 \pi} \int_{B=-\infty}^{B=+\infty} e^{+i B .\left(z-z_{0}\right)} \frac{\delta\left(E-E_{0}\right)}{\Sigma_{t}\left(E_{0}, B\right)} d B & =\frac{\delta\left(E-E_{0}\right)}{2 \pi} \int_{B=-\infty}^{B=+\infty} e^{+i B .\left(z-z_{0}\right)} \frac{\arctan \left(\frac{B}{\Sigma_{t}\left(E_{0}\right)}\right)}{B} d B \\
& =\frac{\delta\left(E-E_{0}\right)}{2} E_{i}\left(\Sigma_{t}\left(E_{0}\right) \cdot\left|z-z_{0}\right|\right)
\end{aligned}
$$

where the complex integral exponential function, $E_{i}$, has been introduced. The analysis of $\Sigma_{t}(E, \vec{B})$ shows that there exist two values (poles) of $\vec{B}$ which render it null, namely $\vec{B}= \pm i \Sigma_{t}(E)$. Moreover, on the purely imaginary axis, the intervals such that $\operatorname{Re}(\vec{B})=0$ and $\operatorname{Im}(\vec{B}) \geq \Sigma_{t}(E)$, make $\Sigma_{t}(E, \vec{B})$ and therefore $\bar{\phi}\left(E, E_{0}, B\right)$ non-analytical. The regular part $\bar{\phi}\left(E, E_{0}, B\right)$ of the flux satisfies the equation:

$$
\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \bar{\phi}\left(E^{\prime}, E_{0}, B\right)-\Sigma_{t}(E, B) \bar{\phi}\left(E, E_{0}, B\right)+\frac{\Sigma_{s}\left(E_{0} \rightarrow E\right)}{\Sigma_{t}\left(E_{0}, B\right)}=0
$$

This last equation is, strictly speaking, not a Fredholm integral equation (because of the multiplicative term $\Sigma_{t}(E, B)$ ), but it can be expressed in that way through an intelligent change of variable, which serves to remove the multiplicative term, by introducing:

$$
\begin{gathered}
\psi_{B}(E) \equiv \sqrt{\Sigma_{t}(E, B)} \frac{\bar{\phi}(E, B)}{\sqrt{m(E)}} \\
G_{B}\left(E^{\prime}, E\right) \equiv \sqrt{\frac{m\left(E^{\prime}\right)}{m(E)}} \frac{\Sigma_{t}\left(E^{\prime} \rightarrow E\right)}{\sqrt{\Sigma_{t}\left(E^{\prime}, B\right) \Sigma_{t}(E, B)}} \\
S_{B}(E) \equiv \frac{\frac{\Sigma_{s}\left(E_{0} \rightarrow E\right)}{\Sigma_{t}\left(E_{0}, B\right)}}{\sqrt{m(E) \Sigma_{t}(E, B)}}
\end{gathered}
$$

Fig. 8.30 Representation of the complex plan and non-analytic zones of the flux, as well as a visualization of the integration path for complex integrals (from Guasp 1970)

where $m(E)$ is Maxwell's function. With these changes of variables, the equation is then written:

$$
\begin{equation*}
\int_{0}^{\infty} d E^{\prime} G_{B}\left(E^{\prime}, E\right) \psi_{B}\left(E^{\prime}\right)-\psi_{B}(E)+S_{B}(E)=0 \tag{8.53}
\end{equation*}
$$

where $G_{B}\left(E^{\prime}, E\right)=G_{B}\left(E, E^{\prime}\right)$ if $B$ is real or purely imaginary, with a magnitude smaller than $\Sigma_{t}(E)$, i.e., the usual micro-reversibility property only applicable in thermalization region. On the other hand, if $B$ is an arbitrary complex number, the micro-reversibility property is not ensured. Through a rigorous mathematical analysis, Guasp shows that the regular function $\bar{\phi}\left(E, E_{0}, B\right)$ is analytic except for a discrete spectrum of purely imaginary eigenvalues $\pm i B_{k}$ and for a continuous spectrum of purely imaginary values such that $\operatorname{Im}(\vec{B}) \geq \Sigma_{t}(E)$.

The eigenvalues of the discrete spectrum are those that allow a non-trivial solution to Eq. 8.53. Knowing the non-analytical domain of the function $\bar{\phi}\left(E, E_{0}, B\right)$ allows the construction of an integration path which excludes the poles of the complex integral, which enables the evaluation of the integral over $B$ through the residue theorem. It should be noted that all the eigenvalues of the problem are on the purely imaginary axis. Guasp also proposed an easily programmable variational method to evaluate the discrete eigenvalues. These eigenvalues correspond to the poles of the Fourier transform of the Green's function. These poles introduce, in the solution of the flux, terms which decrease exponentially with respect to the distance from neutron source (Fig. 8.30).

The work of Guasp is an extremely interesting generalization of the seminal work of Case and of Millot on the $1 D$ Boltzmann equation, and on the exponential attenuation with respect to the distance from the source, which will be later analyzed.

### 8.7 The 1D Transport Equation

### 8.7.1 General Points

In the particular simple case of $1 D$ geometry (suppose the $\vec{x}$ axis in Cartesian geometry), the transport equation can be considerably simplified. This situation, while not necessarily realistic, however helps to properly understand the underlying physics, with an alleviated notation. It will be assumed that the flux has a rotational symmetry about the $\vec{x}$ axis and that the differential scattering cross section depends only on the scalar product, $\vec{\Omega} \cdot \vec{\Omega}^{\prime}$, of the angles before and after the collision. It has been seen that this assumption is not completely exact for crystalline media (Fig. 8.31).

Usually, the cosine of the angle between the vector $\vec{\Omega}$ and the $\vec{x}$ axis is denoted by $\mu=\vec{\Omega} \cdot \vec{x}=\cos \theta$. One should be careful to realize that the angle $\theta$ does not correspond to the angle between the directions before and after the collision. In this geometry, the flux depends only on the $x$ coordinate and $\mu$ :

$$
\Phi(x, \mu)=n(x, \mu) v=2 \pi \Phi(x, \vec{\Omega})
$$

The integrated flux is given by the equation:

$$
\Phi(x) \equiv \int_{-1}^{+1} \Phi(x, \mu) d \mu
$$

In Cartesian geometry, the first term of the transport equation:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E, \vec{\Omega})=\mu \frac{\partial \Phi}{\partial x}+\eta \frac{\partial \Phi}{\partial y}+\xi \frac{\partial \Phi}{\partial z}
$$

simplifies to $\mu \partial \Phi(x, \mu, E) / \partial x$ in the $1 D$ geometry case. The $1 D$ Boltzmann equation is then written:

Steady-state Boltzmann equation in $1 D$ :
$\mu \frac{\partial \Phi(x, \mu, E)}{\partial x}+\Sigma_{t}(x, E) \Phi(x, \mu, E)=\int_{0}^{\infty} d E^{\prime} \int_{-1}^{+1} \Sigma_{S}\left(x, \mu^{\prime} \rightarrow \mu, E^{\prime} \rightarrow E\right) \Phi\left(x, \mu^{\prime}, E^{\prime}\right) d \mu^{\prime}+S(x, \mu, E)$

Fig. 8.31 Angular representation for the $1 D$ transport equation


The limits of the integral of the scattering source term correspond to the limit values of the cosine, for an integration over the whole space. Integrating Eq. 8.54 over energy leads to the Boltzmann equation with an integrated flux:

$$
\mu \frac{\partial \Phi(x, \mu)}{\partial x}+\Sigma_{t}(x) \Phi(x, \mu)=\int_{-1}^{+1} \Sigma_{S}\left(x, \mu^{\prime} \rightarrow \mu\right) \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}+S(x, \mu)
$$

If the medium is not absorbing, the total cross section is replaced by the scattering cross section. In the case where the scattering is isotropic, the differential scattering cross section simplifies:

$$
\Sigma_{S}\left(x, \mu^{\prime} \rightarrow \mu\right)=\frac{1}{2} \Sigma_{S, 0}(x)
$$

We then look for a solution of the flux in the form:

$$
\Phi(x, \mu)=a x+b \mu+c .
$$

Substituting that into the differential equation, we find:

$$
\mu a+\Sigma_{s}(x)(a x+b \mu+c)=\frac{1}{2} \Sigma_{s}(x)[(a x+c) \mu]_{\mu=-1}^{\mu=+1}=\Sigma_{s}(x)(a x+c)
$$

which is valid only if $b=-a / \Sigma_{s}(x)$. A general solution to a problem without absorption or source has thus been found:

Angular flux in a non-absorbing medium without source:

$$
\begin{equation*}
\Phi(x, \mu)=a\left(x-\frac{\mu}{\Sigma_{s}(x)}\right)+c \tag{8.55}
\end{equation*}
$$

where parameters $a$ and $c$ are constants. Since the flux has to be positive, this expression is physically meaningful only for a set of coefficients satisfying that condition. Regarding the integrated flux, it is:

$$
\Phi(x)=\int_{-1}^{+1} \Phi(x, \mu) d \mu=2(a x+c)
$$

It is one of the very rare situations where an analytical expression can be found for the angular flux of the Boltzmann equation. Indeed, even the problem of neutron diffusion in an infinite medium in plane geometry, with constant cross sections and completely elastic collisions, still does not have an exact analytical solution yet but only asymptotic solutions valid for some range of values of distance and energy ${ }^{46}$ while the restrictive assumptions might have led to believe that the problem is simple.

[^173]Fig. 8.32 Spherical coordinates used for the Boltzmann equation


In spherical geometry, care should be taken to not confuse the angle $\theta$ of collision previously defined with the angle $\theta$ usually used for the second spherical coordinate (in $(r, \theta, \varphi)$ ). The deviation angle here is represented by the angle $\chi$ between the vector $\vec{r}$ and the vector $\vec{\Omega}$. Since the notation $\theta$ is retained for the co-latitude in spherical coordinates, the cosine of the collision angle is therefore $\mu=\cos \chi$. If we consider a neutron going in a straight line along the path $\ell \vec{\Omega}$, the Boltzmann equation involves the derivative with respect to the variable $\ell$ along the neutron path:
$\frac{\partial \Phi(\vec{r}, \vec{\Omega})}{\partial \ell}+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})=\int \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}+S(\vec{r}, \vec{\Omega})=Q(\vec{r}, \vec{\Omega})$
It therefore seems that $\frac{d}{d \ell}=\vec{\Omega} \cdot \overrightarrow{g r a d}$.
For spherical coordinates the flux gradient is thus given by Lewis and Miller (1993, p29):

$$
\frac{\partial \Phi}{\partial \ell}=\frac{\partial \Phi}{\partial r} \frac{d r}{d s}+\frac{\partial \Phi}{\partial \mu} \frac{d \mu}{d s}=\frac{\partial \Phi}{\partial r} \mu+\frac{\partial \Phi}{\partial \mu} \frac{d \mu}{d \chi} \frac{d \chi}{d s}
$$

Noticing that, by construction, (Fig. 8.32), $\frac{d r}{d \ell}=\mu=\cos \chi$ and $\sin \chi=-r \frac{d \chi}{d \ell}$, we have:

$$
\frac{d \mu}{d \ell}=\frac{1-\mu^{2}}{r}
$$

The transport equation in one-dimensional spherical geometry is finally written:

Boltzmann equation in $1 D$ spherical geometry:

$$
\begin{align*}
& \mu \frac{\partial \Phi(\vec{r}, \mu)}{\partial r}+\left(\frac{1-\mu^{2}}{r}\right) \frac{\partial \Phi(\vec{r}, \mu)}{\partial \mu} \Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega}) \\
& \quad=\int \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}+S(\vec{r}, \vec{\Omega})=Q(\vec{r}, \vec{\Omega}) \tag{8.56}
\end{align*}
$$

Some authors at times write the gradient term in the form termed conservative, i.e.:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \mu)=\frac{\mu}{r^{2}} \frac{\partial r^{2} \Phi(\vec{r}, \mu)}{\partial r}+\frac{\partial\left(\frac{1-\mu^{2}}{r}\right) \Phi(\vec{r}, \mu)}{\partial \mu}
$$

If higher dimensional spherical geometries are considered, the equations become substantially more complex and involve the different angles in Fig. 8.32. Lewis and Miller (1993), in particular, gives the analytical expressions for the gradient term in different cylindrical and spherical configurations.

### 8.7.2 Lafore and Millot Method, Case Method

### 8.7.2.1 Historical Overview

The homogeneous $l D$ transport equation is written

$$
\mu \frac{\partial \Phi(x, \mu)}{\Sigma_{t} \partial x}+\Phi(x, \mu)=\frac{c}{2} \int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}
$$

where parameter $c$ is the average number of secondary neutrons per collision:

$$
c \equiv \frac{\Sigma_{s}+v \Sigma_{f}}{\Sigma_{t}}
$$

This equation will be rewritten using a change of variable for space, namely, $\mathrm{x}=\Sigma_{t} x$ (which is equivalent to considering distance in transport mean free paths):

$$
\mu \frac{\partial \Phi(\mathrm{x}, \mu)}{\partial \mathrm{x}}+\Phi(\mathrm{x}, \mu)=\frac{c}{2} \int_{-1}^{+1} \Phi\left(\mathrm{x}, \mu^{\prime}\right) d \mu^{\prime}
$$

It is thanks to Lafore and Millot, ${ }^{47}$ as from early as 1958, ${ }^{48}$ and probably independently thanks to Kenneth M. Case, as from

[^174]
(Courtesy Lafore)
Jean-Paul Millot (1934-2001) graduated from the "Ecole Normale Supérieure" in 1953 where he was the student of Professor Schwartz, whose works in distribution theory he used in his thesis. After an extremely innovative State Ph.D. on solving the Boltzmann equation in 1962 (Etude de la diffusion des neutrons rapides, Section efficace de déplacement [On the study of scattering of fast neutrons, ]) at Fontenay aux Roses (on the suburbs of Paris-site where the first French reactor Zoé was built), he worked at the CEA in Cadarache (France) where he would describe the CABRI reactor and conceive the PHEBUS reactor. He would then move to Framatome in 1970. Jean-Paul Millot spent the majority of his career in Framatome where he was Head of the Neutronics Department and then Head of the Reactor Core Department around 1980. A very innovative person, he is credited with the first designs of Framatome outside the bounds of the Westinghouse license. In particular, he is an advocate of control rod mode " G " for "grey", and also of algorithms for protection chains of P4 and N4 designs. He then became Head of the High-Converting Spectral Shift Reactor (Réacteur Convertible à Variation de Spectre (RCVS)) project-a novel PWR concept without boron where the control was only through the control rods.


[^175]$1960,{ }^{49}$ that the idea of looking for solutions to the $1 D$ case in the form below arose:
$\Phi(\mathrm{x}, \mu)=\Phi_{\nu}(\mu) e^{-\frac{\mathrm{x}}{\nu}}$ in Case notations, which are usually used nowadays.
This separation of variables involving an exponential term is suggested by the translation invariance of the homogeneous $l D$ transport equation. Lafore and Millot instead use, since 1958 , the notation $\Phi(x, \mu)=e^{-\alpha x} g(\alpha, \mu)$ where $\alpha \equiv \frac{1}{\nu}$ and show that the functions $g(\alpha, \mu)$ have the form:
$$
g(\alpha, \mu)=\frac{\Sigma_{s}}{\Sigma_{t}-\alpha \mu}+K(\alpha) \delta\left(\Sigma_{t}-\alpha \mu\right)
$$

They prove that these functions are orthogonal when they are associated with the product:

$$
\int_{-1}^{+1} \mu g_{1}\left(\alpha_{1}, \mu\right) g_{2}\left(\alpha_{2}, \mu\right) d \mu=\delta\left(\alpha_{1}-\alpha_{2}\right) \Theta\left(\alpha_{1}\right)
$$

where $\Theta\left(\alpha_{1}\right)$ is a function computed by Millot for the discrete-value solutions, $\alpha_{0}$, of the dispersion equation:

$$
\Theta\left(\alpha_{0}\right)=\frac{\Sigma_{s}^{2}}{\alpha_{0}}\left[\frac{\Sigma_{t}}{\Sigma_{t}^{2}-\alpha_{0}^{2}}-\frac{1}{\Sigma_{s}}\right]
$$

and for the continuous spectrum:

$$
\Theta(\alpha)=\frac{\Sigma_{s}^{2}}{\alpha}\left[\pi^{2}-\left(\frac{\alpha}{\Sigma_{s}}+\ln \left(\left|\frac{\Sigma_{t}+\alpha}{\Sigma_{t}-\alpha}\right|\right)\right)^{2}\right]
$$

[^176]A particularly seminal point in 1962, year of the completion of Millot's thesis, is the demonstration of the completeness of the basis set of functions $g(\alpha, \mu)$ with respect to sufficiently regular functions, as is shown by the use of the notation:

$$
f(\mu)=\sum g(\alpha, \mu) A(\alpha)
$$

where $\sum$ is an integral $\left(\int_{\alpha} d \alpha\right)$ for $|\alpha|>\Sigma_{t}$ and a discrete sum for the two real values $\pm \alpha_{0}$.

In this article of 1960, Case refers to the works ${ }^{50}$ of N. G. Van Kampen ${ }^{51}$ who studied the oscillations of electron plasmas in steady-state. In this type of problem, Anatoly Vlasov (1908-1975) showed that stationary plane waves could be solutions to the linearized transport equation, if the wave vector $\kappa$ and the frequency $\omega$ were the solution of a dispersion equation of the form (with $f_{0}(v)$ the speed distribution at equilibrium):

$$
\frac{4 \pi e^{2}}{m} n_{0} \frac{\kappa}{k} \int \frac{\partial f_{0}}{\partial v} \frac{d v}{\kappa v-\omega}=1
$$

[^177]
(The Marguet collection, Photograph unknown)

This equation is of the same form as the dispersion equation in neutronics. It was Van Kampen who, in 1955, suggested evaluating this integral using the Cauchy principal value method, and expressing the solution with an expansion using a continuous spectrum of functions, contrary to the Lev Landau's ${ }^{52}$ approach, who considered the problem using a Laplace transform. Case was very up-to-date with this work since he himself studied the problem of plasma oscillations in an article in $1959,{ }^{53}$ which shows that the approaches of Van Kampen and Landau are equivalent.

[^178]
(Public domain)
${ }^{53}$ Kenneth M. Case: Plasma oscillations, Annals of Physics, Vol. 9, pp349-364 (1959).

### 8.7.2.2 Theory

By introducing the form of the flux in the equation, we find:

$$
(\nu-\mu) \Phi_{\nu}(\mu)=\frac{c \nu}{2} \int_{-1}^{+1} \Phi_{\nu}\left(\mu^{\prime}\right) d \mu^{\prime}
$$

Dividing by $(\nu-\mu)$, when it is valid (i.e., $\nu \neq \mu)$, and then integrating over $\mu \in[-1,1]$, the dispersion equation (8.46) is recovered, then written with K. M. Case's notation in the form:

Dispersion equation with Case notations:

$$
\begin{equation*}
A(\nu)=1-\frac{c \nu}{2} \oint_{[-1,+1]} \frac{1}{\nu-\mu} d \mu=1-\frac{c \nu}{2} \operatorname{In}\left(\frac{\nu+1}{\nu-1}\right)=0 \quad \text { with } \nu=\frac{\Sigma_{t}}{B} \tag{8.57}
\end{equation*}
$$

The integral symbol $\oint_{[-1,+1]}$ represents an integration over $[-1,+1]$ in the sense of Cauchy's principle value, to take into account the case where $\nu \in[-1,+1]$. There are solutions for two discrete eigenvalues $\pm \nu_{0}$ (of opposite sign), which are solutions to the dispersion equation, as we have seen previously, and whose related normalized eigenvectors are given by:

$$
\Phi_{0}^{ \pm}(\mu)= \pm \frac{c \nu_{0}}{2} \frac{1}{\left( \pm \nu_{0}-\mu\right)}
$$

However, Case, like Lafore and Millot, noticed that there were also as solution all functions for any $\nu \in[-1,1]$, constructed in the form:

Continuous spectrum of Case's eigenvectors:

$$
\begin{equation*}
\Phi_{\nu}(\mu)=\frac{c \nu}{2} \frac{1}{(\nu-\mu)}+\lambda(\nu) \delta(\nu-\mu) \tag{8.58}
\end{equation*}
$$

with $\lambda(\nu) \equiv\left(A^{+}(\nu)+A^{-}(\nu)\right) / 2$ and $A^{ \pm}(\nu) \equiv \lim _{\varepsilon \rightarrow 0}(A(\nu \pm i \varepsilon))$, i.e., the Cauchy definition of the principal value. The distribution $\delta(\nu-\mu)$ is defined by:

$$
\oint_{[-1,+1]} \delta(\nu-\mu) F(\mu) d \mu= \begin{cases}F(\nu) & \text { if } \nu \in[-1,+1] \\ 0 & \text { otherwise }\end{cases}
$$

Case named these functions the continuous spectrum of eigenvectors, much to mathematicians ${ }^{54}$ chagrin. These eigenvectors are arbitrarily normalized to 1 , which can be verified by evaluating:

$$
\int_{-1}^{+1} \Phi_{\nu}(\mu) d \mu=\frac{c \nu}{2} \oint_{[-1,+1]} \frac{1}{(\nu-\mu)} d \mu+\lambda(\nu)=1
$$

using the very definition of $\lambda(\nu)$. The functions $\Phi_{\nu}(\mu) e^{-\frac{x}{\nu}}$ are, by construction, all solutions of the homogeneous transport equations. Finally, Case gives the general solution as a combination of three solutions: the two discrete ones and the one from the continuous spectrum:

[^179]

Paul Zweifel

$$
\Phi(\mathrm{x}, \mu)=a_{0}^{+} \Phi_{0}^{+}(\mu) e^{-\frac{x}{\nu_{0}}}+a_{0}^{-} \Phi_{0}^{-}(\mu) e^{+\frac{x}{\nu_{0}}}+\int_{-1}^{+1} f(\nu) \Phi_{\nu}(\mu) e^{-\frac{x}{\nu}} d \nu
$$

The constants $a_{0}^{+}, a_{0}^{-}$and the function $f(\nu)$ are defined through the boundary conditions. We will be coming back to Case's method in more detail, in the albedo problem in the next chapter. We can generalize this approach to a lattice of $m$ homogeneous plates by taking into account the anisotropy. ${ }^{55}$ The $1 D$ Boltzmann equation accounting for anisotropy will be written by expanding the scattering and fission terms with Legendre polynomials-method which will be described in detail in Chap. 9:

$$
\mu \frac{\partial \Phi(\mathrm{x}, \mu)}{\partial \mathrm{x}}+\Phi(\mathrm{x}, \mu)=\frac{c}{2} \sum_{l=0}^{n} b_{l} P_{l}(\mu) \int_{-1}^{+1} P_{l}\left(\mu^{\prime}\right) \Phi\left(\mathrm{x}, \mu^{\prime}\right) d \mu^{\prime}
$$



Paul Zweifel and the reference text on neutron transport (The Marguet collection)
${ }^{55}$ J. Kenneth Shultis: A new method for the calculation of the emergent distributions for the anisotropic slab albedo problem, Journal of Computational Physics, Vol. 11, n ${ }^{\circ} 1,109-126$ (1973).

The solution is written:

$$
\Phi(\mathrm{x}, \mu)=\sum_{j=1}^{m} a_{j}^{+} \Phi_{j}^{+}(\mu) e^{-\frac{\mathrm{x}}{\nu_{j}}}+\sum_{j=1}^{m} a_{j}^{-} \Phi_{j}^{-}(\mu) e^{+\frac{\mathrm{x}}{\nu_{j}}}+\int_{-1}^{+1} f(\nu) \Phi_{\nu}(\mu) e^{-\frac{\mathrm{x}}{\nu}} d \nu
$$

where the coefficients $a_{j}^{+}, a_{j}^{-}$and $f(\nu)$ depend on the boundary conditions and where the $m$ pairs of eigenvalues $\pm \nu_{j}\left(1 \leq m \leq n+1,\left|\nu_{j}\right|>1\right)$ are the solutions to the dispersion equation:

$$
1-\frac{c \nu}{2} \oint_{[-1,+1]} \frac{D(\mu, \mu)}{(\nu-\mu)} d \mu=1 \quad \text { with: } \quad D(\nu, \mu)=\sum_{l=0}^{n} b_{l} h_{l}(\nu) P_{l}(\mu)
$$

where coefficients $h_{l}(\mu)$ are given by the iteration equation:

$$
(l+1) h_{l+1}(\mu)-\nu\left(2 l+1-b_{l} c\right) h_{l}(\mu)+l h_{l-1}(\mu) \quad \text { with } h_{0}(\mu) \equiv 1
$$

The discrete eigenvectors are given by:

$$
\Phi_{j}^{ \pm}(\mu)=\frac{c \nu_{j}}{2} \frac{D\left(\nu_{j}, \pm \mu\right)}{\left(\nu_{j} \mp \mu\right)} \quad j=1, \cdots, m
$$

On the other hand, the continuous spectrum eigenvectors are given by:

$$
\Phi_{\nu}(\mu)=\frac{c \nu}{2} \frac{D(\nu, \mu)}{(\nu-\mu)}+\lambda(\nu) \delta(\nu-\mu) \quad \text { with: } \lambda(\nu)=1-\frac{c \nu}{2} \oint_{[-1,+1]} \frac{D(\mu, \mu)}{(\nu-\mu)} d \mu
$$

The continuous spectrum and discrete eigenvectors satisfy the orthogonality property:

$$
\int_{-1}^{+1} \mu \Phi_{\nu}(\mu) \Phi_{\nu^{\prime}}(\mu) d \mu=\left\{\begin{array}{l}
v\left(\lambda^{2}(\nu)+\left(\frac{c \pi \nu}{2} D(\nu, \nu)\right)^{2}\right) \text { for } \nu=\nu^{\prime} \\
0 \text { if } \nu \neq \nu^{\prime} \text { for } \nu \in[-1,+1], \nu^{\prime} \in[-1,+1], \text { or for } \pm \nu_{j}
\end{array}\right.
$$

and:

$$
\int_{-1}^{+1} \mu\left(\Phi_{j}^{ \pm}(\mu)\right)^{2} d \mu= \pm \frac{c \nu_{j}^{2}}{2} \int_{-1}^{+1} \frac{D^{2}\left(\nu_{j}, \nu\right)}{\left(\nu_{j}-\mu\right)^{2}}
$$

These orthogonality relations are useful for finding the coefficients $a_{j}^{+}, a_{j}^{-}$and $f(\nu)$, depending on the type of problem considered (Shultis evaluated these in the case of collimated or pencil beam of particles for Fredholm's ${ }^{56}$ equation with $c \leq 1$ ). Garcia and Siewert generalized ${ }^{57}$ this approach in multi-group for a transfer, in the form of a triangular matrix. Finally in 1992, Garis, Pazsit and Sahni developed ${ }^{58}$ the complete solution of the plane critical monokinetic problem with two regions $c_{1}$ and $c_{2}$. They showed that the spectrum of the eigenvalues consisted of continuous lines in the plane $c_{1} \otimes c_{2}$, which never coupled with each other. We show that, for some discrete values of $c_{1}>1, c_{2}$ diverges to $-\infty$.

### 8.7.3 Perovich Method

In 1997, S. Perovich proposed ${ }^{59}$ an elegant solution, completely analytical in the case $c \in[0,1]$, by solving the transcendental equation:

[^180]
(Public domain)
${ }^{57}$ R.D.M. Garcia, C.E. Siewert: Mulstislab multi-group transport theory with $L^{\text {th }}$ order anisotropic scattering, Journal of Computational Physics, Vol. 50, n ${ }^{\circ} 1$, 181-192 (1983).
${ }^{58}$ N.S. Garis, I. Pazsit, D.C. Sahni: Generalization of the eigenvalue problem of the one-speed neutron transport equation in two-region systems, Progress in nuclear energy, Vol. 27, n ${ }^{\circ} 4$, 305-334 (1992).
${ }^{59}$ S.M. Perovich: Concerning the analytical solution of the dispersion equation in the linear transport theory, Transport Theory and Statistical Physics, 26 (6), 705-725 (1997).
$$
Z=\frac{e^{f Z}-1}{e^{f Z}+1} \text { with } Z=\frac{1}{\nu} \text { and } f=\frac{2}{c}
$$
whose unique solution is given in the form:
$Z_{0}=\frac{1}{f} \log \left(\frac{T(t-f)}{T(t)}\right)$ for $t>t_{0}, f \in[2, \infty[$ and where:
\[

\left\{$$
\begin{array}{l}
T(t)=\left(N(t)+\frac{d N(t)}{d t}\right) e^{t} \\
N(t)=\left\{\begin{array}{l}
\sum_{n=0}^{E\left[\frac{t}{f}\right]}(-1)^{n} e^{-n f} \sum_{k=0}^{k=n} \frac{2^{k}(t-n f)^{k} n!}{(k!)^{2}(n-k)!} \text { for } t>0 \\
0 \quad \text { for } t<0
\end{array}\right.
\end{array}
$$\right.
\]

The solutions $\nu_{0}^{ \pm}$of Case's dispersion equation are then written:

$$
\nu_{0}^{ \pm}= \pm \frac{1}{\frac{1}{f} \operatorname{In}\left(\frac{T(t-f)}{T(t)}\right)}
$$

These results, stated here without proof, show that the solution, while analytical, remains very complex.

### 8.8 Asymptotic Solution for Diffusion

(Neutron thermalization 1962)

### 8.8.1 Exponential Relaxation of the Flux, Far from the Source

In the case of a poorly-absorbing medium and in a region far away from sources, there exists an asymptotic solution to the monokinetic transport equation, which satisfies a diffusion equation. In an infinite medium, the asymptotic flux solution is the solution to the transport equation, so far as, very far away from the source, it can be expected that the neutrons would have all undergone several collisions (Bekurts
and Wirtz 1964, p89). Consider the monoenergetic transport equation in a homogeneous isotropic medium without source terms:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t} \Phi(\vec{r}, \vec{\Omega})=\frac{1}{4 \pi} \Sigma_{S} \int_{4 \pi} \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}
$$

We will look for a solution $\Phi(\vec{r}, \vec{\Omega})$ in the form $\phi(\vec{\Omega}) e^{-\kappa r}$ (Barjon 1993). $1 / \kappa$ is, in fact, the thermal diffusion length-and is also going to be the eigenvalue of the transport equation, corresponding to the eigenvector $\phi(\vec{\Omega}) e^{-\kappa r}$ (Nelkin in (Neutron thermalization, 1962 pRF-5)). The perfect analogy with the Fourier transform seen previously should be noted. By introducing this form in the transport equation (one-dimensional to simplify calculations), and using the cosine, $\mu$, of the collision angle, we can write the implicit equation which governs the behavior of the angular part of the flux:

$$
\left(-\mu \kappa+\Sigma_{t}\right) \varphi(\mu)=\frac{\Sigma_{s}}{2} \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) d \mu^{\prime}
$$

$\varphi(\mu)$ can then be integrated over $[-1,+1]$ to obtain an equation independent of the flux:

$$
\int_{-1}^{+1} \varphi(\mu) d \mu=\frac{\Sigma_{s}}{2} \int_{-1}^{+1} \frac{1}{\left(-\mu \kappa+\Sigma_{t}\right)} d \mu \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) d \mu^{\prime}
$$

whose only solution is that the constant $\kappa$ satisfies the transcendental equation:

$$
\begin{equation*}
\int_{-1}^{+1} \frac{1}{\left(-\mu \kappa+\Sigma_{t}\right)} d \mu=\frac{2}{\Sigma_{s}} \quad \text { or: } \quad \ln \left(\frac{1+\frac{\kappa}{\Sigma_{t}}}{1-\frac{\kappa}{\Sigma_{t}}}\right)=\frac{2 \kappa}{\Sigma_{s}} \tag{8.59}
\end{equation*}
$$

The linear attenuation coefficient $\kappa$ varies continuously, from $\Sigma_{t}$, when there is no scattering but only absorption, i.e., $\Sigma_{t}=\Sigma_{a}$, to zero when $\Sigma_{a}=0$. The case $\kappa<0$ does not have any physical meaning since the flux would tend to infinity. As for the function $\varphi(\mu)$, it is defined up to a multiplicative constant, by:

$$
\varphi(\mu)=\frac{\Sigma_{s}}{\left(\Sigma_{t}-\mu \kappa\right)}
$$

Finally, the angular flux is given by:

$$
\Phi(x, \mu)=\frac{\Sigma_{s}}{4 \pi\left(\Sigma_{t}-\mu \kappa\right)} \alpha e^{-\kappa x}
$$

The coefficient $4 \pi$ has been introduced so as to satisfy the total flux equation, integrated over $4 \pi$ steradians:

$$
\Phi(x)=2 \pi \int_{-1}^{+1} \Phi(x, \mu) d \mu=\alpha e^{-\kappa x}
$$

which satisfies the diffusion equation: $\Delta \Phi(x)-\kappa^{2} \Phi(x)=0$. On the other hand, we can show that the neutron current obeys Fick's law with $D=\Sigma_{a} / \kappa^{2}$ :

$$
J(x)=2 \pi \int_{-1}^{+1} \Phi(x, \mu) \mu d \mu=\frac{\Sigma_{a}}{\kappa} \alpha e^{-\kappa x}=-D\|\overrightarrow{\operatorname{grad}} \Phi(x)\|
$$

In case where $\kappa / \Sigma_{t}$ is small compared to 1 (i.e. $\Sigma_{a}$ small compared to $\Sigma_{s}$ ), we can find the value of $\kappa$ by expanding Eq. 8.59 using a power series:

$$
\ln \left(\frac{1+\frac{\kappa}{\Sigma_{t}}}{1-\frac{\kappa}{\Sigma_{t}}}\right)=2\left(\frac{\kappa}{\Sigma_{t}}+\frac{1}{3}\left(\frac{\kappa}{\Sigma_{t}}\right)^{3}+\frac{1}{5}\left(\frac{\kappa}{\Sigma_{t}}\right)^{5}+\ldots\right)=\frac{2 \kappa}{\Sigma_{s}}
$$

leading to: $1+\frac{1}{3}\left(\frac{\kappa}{\Sigma_{t}}\right)^{2}+\frac{1}{5}\left(\frac{\kappa}{\Sigma_{t}}\right)^{4}+\ldots=\frac{\Sigma_{t}}{\Sigma_{s}}=1+\frac{\Sigma_{a}}{\Sigma_{s}}$
which will be expanded up to a quartic function in $\kappa / \Sigma_{t}:\left(\frac{\kappa}{\Sigma_{t}}\right)^{4}+$ $\frac{5}{3}\left(\frac{\kappa}{\Sigma_{t}}\right)^{2}-5 \frac{\Sigma_{a}}{\Sigma_{s}}=0$.
which has as only positive root: $\left(\frac{\kappa}{\Sigma_{t}}\right)^{2}=\frac{-\frac{5}{3}+\sqrt{\left(\frac{5}{3}\right)^{2}-20 \frac{\Sigma_{a}}{\Sigma_{s}}}}{2} \approx 3 \frac{\Sigma_{a}}{\Sigma_{s}}\left(1-\frac{9 \Sigma_{a}}{5}\right)$
Hence, by using $\Sigma_{t}=\Sigma_{a}+\Sigma_{s}$ :

$$
\kappa^{2} \approx 3 \frac{\Sigma_{a} \Sigma_{t}^{2}}{\Sigma_{t}-\Sigma_{a}}\left(1-\frac{9}{5} \frac{\Sigma_{a}}{\Sigma_{t}-\Sigma_{a}}\right) \approx 3 \Sigma_{a} \Sigma_{t}\left(1-\frac{4}{5} \frac{\Sigma_{a}}{\Sigma_{t}}-\frac{13}{5}\left(\frac{\Sigma_{a}}{\Sigma_{t}}\right)^{2}+O\left(\frac{\Sigma_{a}}{\Sigma_{t}}\right)^{3}\right)
$$

The diffusion coefficient can thus be obtained (Bonilla 1957, p186; Etherington 1957, p6-35):

$$
D=\frac{\Sigma_{a}}{\kappa^{2}} \approx \frac{1}{3 \Sigma_{t}\left(1-\frac{4}{5} \frac{\Sigma_{a}}{\Sigma_{t}}-\frac{13}{5}\left(\frac{\Sigma_{a}}{\Sigma_{t}}\right)^{2}+\ldots\right)}
$$

If a $P_{1}$ expansion of the scattering cross section is considered, it yields:

$$
\Sigma_{s}\left(\mu_{0}\right)=\frac{1}{2} \sum_{l=0}^{l=1}(2 l+1) \Sigma_{s, l} P_{l}\left(\mu_{0}\right)=\frac{1}{2} \Sigma_{s, 0}+\frac{3}{2} \mu_{0} \Sigma_{s, 1}
$$

with $\Sigma_{s, 1}=\int_{-1}^{+1} P_{1}\left(\mu_{0}\right) \Sigma_{s}\left(\mu_{0}\right) d \mu_{0}=\int_{-1}^{+1} \mu_{0} \Sigma_{s}\left(\mu_{0}\right) d \mu_{0}=\overline{\mu_{0}} \quad \Sigma_{s, 0}$. Using the addition theorem of Legendre polynomials, and realizing that the angular integration of the complementary term having the associated Legendre polynomials is zero, we have:

$$
\begin{aligned}
\int_{4 \pi} \Sigma_{s}\left(\vec{\Omega}^{\prime} \cdot \vec{\Omega}\right) \Phi\left(\vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} & =\int_{-1}^{+1}\left(\frac{1}{2} \Sigma_{s, 0}+\frac{3}{2} \mu \mu^{\prime} \Sigma_{s, 1}\right) \Phi\left(\mu^{\prime}\right) d \mu^{\prime} \\
& =\frac{1}{2} \Sigma_{s, 0} \int_{-1}^{+1} \Phi\left(\mu^{\prime}\right) d \mu^{\prime}+\frac{3}{2} \overline{\mu_{0}} \mu \Sigma_{s, 0} \int_{-1}^{+1} \mu^{\prime} \Phi\left(\mu^{\prime}\right) d \mu^{\prime}
\end{aligned}
$$

Substituting this result in the transport equation and carrying out the same procedure as above for the isotropic approximation $P_{0}$, the implicit equation which determines $\kappa$ is found:

$$
\begin{equation*}
\left(-\mu \kappa+\Sigma_{t}\right) \varphi(\mu)=\frac{\Sigma_{s}}{2} \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) d \mu^{\prime}+\frac{3 \overline{\mu_{0}} \Sigma_{s}}{2} \mu \int_{-1}^{+1} \mu^{\prime} \varphi\left(\mu^{\prime}\right) d \mu^{\prime} \tag{8.60}
\end{equation*}
$$

Analyzing this equation, we observe that an angular flux of the form:

$$
\varphi(\mu)=\frac{\alpha_{0}+\alpha_{1} \mu}{\left(\Sigma_{t}-\mu \kappa\right)}
$$

is the solution. Dividing by $\left(\Sigma_{t}-\mu \kappa\right)$ and then integrating over $[-1,+1]$, we find:

$$
\begin{align*}
& \int_{-1}^{+1} \varphi(\mu) d \mu=\int_{-1}^{+1} \frac{1}{\left(\Sigma_{t}-\mu \kappa\right)} d \mu \frac{\Sigma_{s}}{2} \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) d \mu^{\prime}+\frac{3 \overline{\mu_{0}} \Sigma_{s}}{2} \int_{-1}^{+1} \frac{\mu}{\left(\Sigma_{t}-\mu \kappa\right)} d \mu \int_{-1}^{+1} \mu^{\prime} \varphi\left(\mu^{\prime}\right) d \mu^{\prime} \\
& \text { from which: } \quad \frac{1}{\kappa} \ln \left(\frac{1+\frac{\kappa}{\Sigma_{t}}}{1-\frac{\kappa}{\Sigma_{t}}}\right)+3 \overline{\mu_{0}}\left(\frac{\Sigma_{t}}{\kappa^{2}} \ln \left(\frac{1+\frac{\kappa}{\Sigma_{t}}}{1-\frac{\kappa}{\Sigma_{t}}}\right)-\frac{2}{\kappa}\right) \frac{\int_{-1}^{+1} \mu^{\prime} \varphi\left(\mu^{\prime}\right) d \mu^{\prime}}{\int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) d \mu^{\prime}}=\frac{2}{\Sigma_{s}} \tag{8.61}
\end{align*}
$$

This equation, homogeneous over centimeters, differs from Eq. 8.59 by an anisotropy term. Substituting the flux $\varphi(\mu)=\left(\alpha_{0}+\alpha_{1} \mu\right) /\left(\Sigma_{t}-\mu \kappa\right)$ in Eq. 8.60, after identifying the constant terms and the terms in $\mu$ the system of transcendental equations which links $\kappa$ to $\Sigma_{t}$ and $\Sigma_{s}$ is written:

$$
\left\{\begin{array}{l}
\alpha_{0}=\frac{\Sigma_{s}}{2} \alpha_{0} \int_{-1}^{+1} \frac{1}{\left(\Sigma_{t}-\mu \kappa\right)} d \mu+\frac{\Sigma_{s}}{2} \alpha_{1} \int_{-1}^{+1} \frac{\mu}{\left(\Sigma_{t}-\mu \kappa\right)} d \mu \\
\alpha_{1}=\frac{3 \overline{\mu_{0}} \Sigma_{s}}{2} \alpha_{0} \int_{-1}^{+1} \frac{\mu}{\left(\Sigma_{t}-\mu \kappa\right)} d \mu+\frac{3 \overline{\mu_{0}} \Sigma_{s}}{2} \alpha_{1} \int_{-1}^{+1} \frac{\mu^{2}}{\left(\Sigma_{t}-\mu \kappa\right)} d \mu
\end{array}\right.
$$

It can be seen that, by defining $K=\kappa / \Sigma_{t}$, a set of integral functions containing $\mu$ to the $n$th power multiplied by a Legendre polynomial is obtained:

Rational integral of $P_{n}: \quad I P_{l, n}(K) \equiv \int_{-1}^{+1} P_{l}(\mu) \frac{\mu^{n}}{(1-\mu K)} d \mu$

Using this definition, the system is written:

$$
\left\{\begin{array}{l}
\frac{\alpha_{0}}{\alpha_{1}}=\frac{\Sigma_{s}}{2 \Sigma_{t}}\left(\frac{\alpha_{0}}{\alpha_{1}} I P_{0,0}(K)+I P_{0,1}(K)\right) \\
1=\frac{3 \overline{\mu_{0}} \Sigma_{s}}{2 \Sigma_{t}}\left(\frac{\alpha_{0}}{\alpha_{1}} I P_{0,1}(K)+I P_{0,2}(K)\right)
\end{array}\right.
$$

By evaluating the ratio $\alpha_{0} / \alpha_{1}$ using the first equation and substituting it in the second, a transcendental equation in $K$ is obtained:

$$
\frac{2}{3 \overline{\mu_{0}} \Sigma_{s}}=\frac{1}{\Sigma_{t}}\left(\frac{\Sigma_{s}}{2 \Sigma_{t}-\Sigma_{s} I P_{0,0}(K)}\left[I P_{0,1}(K)\right]^{2}+I P_{0,2}(K)\right)
$$

The $I P_{O, n}(K)$ integrals can then be computed analytically, as well as their limited expansions in a power series, assuming $K \ll 1$ :

$$
\left\{\begin{array}{l}
I P_{0,0}(K)=\frac{1}{K} \ln \left[\frac{1+K}{1-K}\right]=2\left(1+\frac{K^{2}}{3}+\frac{K^{4}}{5}+\frac{K^{6}}{7}+O\left(K^{8}\right)\right) \\
I P_{0,1}(K)=\frac{1}{K^{2}} \ln \left[\frac{1+K}{1-K}\right]-\frac{2}{K}=2\left(\frac{K}{3}+\frac{K^{3}}{5}+\frac{K^{5}}{7}+O\left(K^{7}\right)\right) \\
I P_{0,2}(K)=\frac{1}{K^{3}} \ln \left[\frac{1+K}{1-K}\right]-\frac{2}{K^{2}}=2\left(\frac{1}{3}+\frac{K^{2}}{5}+\frac{K^{4}}{7}+O\left(K^{6}\right)\right)=\frac{I P_{0,1}(K)}{K}
\end{array}\right.
$$

By setting: $\delta=\Sigma_{a} / \Sigma_{t}$ and substituting the limited expansion in the transcendental equation, the following is found:
$\frac{1}{3 \overline{\mu_{0}}}=\frac{(1-\delta)^{2}\left(\frac{K}{3}+\frac{K^{3}}{5}+\frac{K^{5}}{7}+O\left(K^{7}\right)\right)^{2}}{1-(1-\delta)\left(1+\frac{K^{2}}{3}+\frac{K^{4}}{5}+\frac{K^{6}}{7}+O\left(K^{8}\right)\right)}+(1-\delta)\left(\frac{1}{3}+\frac{K^{2}}{5}+\frac{K^{4}}{7}+O\left(K^{6}\right)\right)$
It is interesting to note that this equation is an equation in $K^{2}$ which can be transformed by setting $\beta=K^{2} / 3$ and retaining only the terms in $\beta^{2}$, i.e.:

$$
1=\overline{\mu_{0}} \frac{(1-\delta)^{2}\left(\beta+\frac{18}{5} \beta^{2}\right)}{\delta+\beta(\delta-1)+\frac{9}{5} \beta^{2}(\delta-1)}+\overline{\mu_{0}}(1-\delta)\left(1+\frac{9}{5} \beta+\frac{27}{7} \beta^{2}\right)
$$

which will finally be written in the form of a quadratic equation:

$$
\left(1+\frac{15}{7} \overline{\mu_{0}} \delta\right) \beta^{2}+\left(\frac{5}{9}+\overline{\mu_{0}} \delta\right) \beta+\frac{5 \delta}{9}\left(\overline{\mu_{0}}-\frac{1}{1-\delta}\right)=0
$$

We notice that, with the other coefficients positive, the constant is negative for small $x$. The only positive solution is hence given by:

$$
\begin{aligned}
\beta^{+}= & \left.\frac{-\left(\frac{5}{9}+\overline{\mu_{0}} \delta\right)+\sqrt{\left(\frac{5}{9}+\overline{\mu_{0}} \delta\right)^{2}-\left(1+\frac{15}{7} \overline{\mu_{0}} \delta\right) \frac{5 \delta\left(\overline{\mu_{0}}-\frac{1}{1-\delta}\right)}{2\left(1+\frac{15}{7} \overline{\mu_{0}} \delta\right)}}}{} \begin{array}{rl}
(1-\delta)\left(1+\frac{9}{5} \overline{\mu_{0}} \delta\right) & \delta\left(1-\overline{\mu_{0}}+\overline{\mu_{0}} \delta\right) \\
& {\left[1-\frac{\delta\left(1-\overline{\mu_{0}}+\overline{\mu_{0}} \delta\right)\left(1+\frac{15}{7} \overline{\mu_{0}} \delta\right)}{\frac{5}{9}(1-\delta)\left(1+\frac{9}{5} \overline{\mu_{0}} \delta\right)^{2}}+\ldots\right]}
\end{array}\right]
\end{aligned}
$$

Recalling that $\beta=\frac{K^{2}}{3}=\frac{\kappa^{2}}{3 \Sigma_{t}^{2}}=\frac{\Sigma_{a}}{3 \Sigma_{t}^{2} D}=\frac{\delta}{3 \Sigma_{t} D}$, we can calculate the diffusion coefficient obtained through the limited $P_{1}$ expansion of the scattering cross section:

$$
D \approx \frac{1}{3 \Sigma_{t}\left(1-\overline{\mu_{0}}+\overline{\mu_{0}} \delta\right)}(1-\delta)\left(1+\frac{9}{5} \overline{\mu_{0}} \delta\right)
$$

which we will compare to the usual expression for the diffusion coefficient in the $P_{1}$ approximation of the flux and the scattering cross section:

$$
D=\frac{1}{3\left(\Sigma_{t}-\Sigma_{s, 1}\right)}=\frac{1}{3\left(\Sigma_{t}-\overline{\mu_{0}} \Sigma_{s, 0}\right)}=\frac{1}{3 \Sigma_{t}\left(1-\overline{\mu_{0}}+\overline{\mu_{0}} \delta\right)}
$$

This result is found in a different form in (Bekurts and Wirtz 1964, p91). It is noted that the asymptotic flux $\Phi(x, \mu)=e^{-\kappa x}\left(\alpha_{0}+\alpha_{1} \mu\right) /\left(\Sigma_{t}-\mu \kappa\right)$ indeed satisfies a diffusion equation when the diffusion coefficient has the value:

$$
D=\frac{\Sigma_{a}}{3 \Sigma_{t}^{2} \beta}=\frac{1}{3\left(\Sigma_{t}-\Sigma_{s, 1}\right)}
$$

This approach can be generalized if the scattering cross section is expanded to the $n$th order by writing the flux in the form:

$$
\left\{\begin{array}{c}
\Phi(x, \mu)=\varphi(\mu) e^{-\kappa x}=\frac{\sum_{j=0}^{n} \alpha_{i} \mu^{i}}{\left(\Sigma_{t}-\mu \kappa\right)} e^{-\kappa x} \\
\Sigma_{s}\left(x, \mu_{0}\right)=\sum_{l=0}^{n} \frac{2 l+1}{2} \Sigma_{s, l} P_{l}\left(\mu_{0}\right)
\end{array}\right.
$$

Equation 8.60 is then generalized by using the addition theorem of Legendre polynomials already discussed previously:

$$
\sum_{j=0}^{n} \alpha_{i} \mu^{i}=\sum_{l=0}^{n} \frac{2 l+1}{2} \Sigma_{s, l} P_{l}(\mu) \int_{-1}^{+1} P_{l}\left(\mu^{\prime}\right) \frac{\sum_{j=0}^{n} \alpha_{i} \mu^{\prime i}}{\left(\Sigma_{t}-\mu^{\prime} \kappa\right)} d \mu^{\prime}
$$

By introducing the integral functions $I P_{l, j}(K)$, this equation can be written as:

$$
\sum_{j=0}^{n} \alpha_{i} \mu^{i}=\sum_{l=0}^{n} \frac{2 l+1}{2} \frac{\Sigma_{s, l}}{\Sigma_{t}} P_{l}(\mu) \sum_{j=0}^{n} \alpha_{i} I P_{l, j}(K)
$$

Multiplying each term by $P_{k}(\mu)$ and integrating over [ $-1,+1$ ] as described in the methodology developed in $P_{n}$ theory, $n+1$ equations are obtained:

$$
\begin{aligned}
\sum_{j=0}^{n} \alpha_{i} \int_{-1}^{+1} P_{k}(\mu) \mu^{i} d \mu & =\sum_{j=0}^{n} \alpha_{i} I P_{k, j}(0) \\
& =\sum_{l=0}^{n} \frac{2 l+1}{2} \frac{\Sigma_{s, l}}{\Sigma_{t}} \int_{-1}^{+1} P_{k}(\mu) P_{l}(\mu) d \mu \sum_{j=0}^{n} \alpha_{i} I P_{l, j}(K)
\end{aligned}
$$

Using the orthogonality property of Legendre polynomials, a system of linear equations in terms of the flux coefficients is obtained:

$$
\sum_{j=0}^{n} \alpha_{i}\left[I P_{k, j}(0)-\frac{\Sigma_{s, k}}{\Sigma_{t}} I P_{k, j}(\mathrm{~K})\right]=0 \quad k=0, \ldots, n
$$

for which there exists a non-trivial solution if the determinant of the system is zero. The integral functions $I P_{k, j}(K)$ possess the iterative properties associated with Legendre polynomials:

$$
I P_{k, j}(\mathrm{~K})=\frac{k+1}{2 k+1} I P_{k+1, j-1}(\mathrm{~K})+\frac{k}{2 k+1} I P_{k-1, j-1}(\mathrm{~K})
$$

On the other hand, we can calculate $I P_{0, j}(K)$ from integrals of lower orders by noticing that:

$$
\begin{aligned}
-K^{j} I P_{0, j}(K) & =-\int_{-1}^{+1} \frac{(\mu K)^{j}}{(1-\mu K)} d \mu=\int_{-1}^{+1} \frac{1-(\mu K)^{j}}{(1-\mu K)} d \mu-\int_{-1}^{+1} \frac{1}{(1-\mu K)} d \mu \\
& =\sum_{k=0}^{j-1} \int_{-1}^{+1}(\mu K)^{k} d \mu-I P_{0,0}(K)=\sum_{k=0}^{j-1} \frac{\left(1-(-1)^{k+1}\right)}{k+1} K^{k}-I P_{0,0}(K)
\end{aligned}
$$

leading to: $I P_{0, j}(\mathrm{~K})=\frac{1}{\mathrm{~K}^{j}} I P_{0,0}(\mathrm{~K})-\sum_{k=0}^{j-1} \frac{\left(1-(-1)^{k+1}\right)}{k+1} \mathrm{~K}^{k-j}$
Also, using the parity properties of the polynomials $P_{k}(\mu) \mu^{j}$, it can be said that:

$$
I P_{k, j}(0)=\int_{-1}^{+1} P_{k}(\mu) \mu^{j} d \mu=0 \quad \text { if } k+j \text { odd }
$$

Through the iterative formula, the power $j$ of the $\mu^{j}$ can be lowered until $1=P_{0}(\mu)$, which helps to state the following:

$$
I P_{k, j}(0)=0 \quad \text { if } k>j \quad \text { and } \quad I P_{k, k}(0)=\frac{2 k!}{\prod_{j=0}^{k}(2 j+1)}
$$

Together, these properties show that we can compute analytically all the coefficients of the determinant $A(K, n)$ of linear system of angular flux coefficients:

$$
\left|\begin{array}{ccccc}
I P_{0,0}(0)-\frac{\Sigma_{s, 0}}{\Sigma_{t}} I P_{0,0}(K) & I P_{0,1}(0)-\frac{\Sigma_{s, 0}}{\Sigma_{t}} I P_{0,1}(K) & \ldots & \ldots & I P_{0, n}(0)-\frac{\Sigma_{s, 0}}{\Sigma_{t}} I P_{0, n}(K) \\
-\frac{\Sigma_{s, 1}}{\Sigma_{I}}\left(P_{1,0}(K)\right. & I P_{1,1}(0)-\frac{\Sigma_{s, 1}}{\Sigma_{t}} I P_{1,1}(K) & \vdots & & \vdots \\
-\frac{\Sigma_{s, 2}}{\Sigma_{t}} I P_{2,0}(K) & -\frac{\Sigma_{s, 2}}{\Sigma_{t} I P_{2,1}(K)} & I P_{2,2}(0)-\frac{\Sigma_{s, 2}}{\Sigma_{t}} I P_{2,2}(K) & & \\
\vdots & & & \Sigma_{s, n} I P_{n, 0}(K) & \ldots \\
\Sigma_{t} & \ldots & & -\frac{\Sigma_{s, n} I P_{n, n-1}(K)}{\Sigma_{t}} I P_{n, n}(0)-\frac{\vdots}{\Sigma_{s}, n} I P_{n, n}(K)
\end{array}\right|
$$

The transcendental equation $A(K, n)=0$ gives the value of $K=\kappa / \Sigma_{t}$ (at least numerically, thanks to root-finding algorithms, if the determinant is developed-see (Durand 1960; Traub 1964)), describing the spatial part of asymptotic diffusion flux. The method can be generalized to a finite medium by taking into account two spatial components: $e^{-\kappa x}$ and $e^{+\kappa x}$. The introduction of positive exponentials can be considered by using $I P_{k, j}(-K)$, knowing that:

$$
I P_{k, j}(-K)=(-1)^{k+j} I P_{k, j}(K)
$$

The asymptotic flux is even more rapidly reached for low absorption ( $\delta \ll 1$ ) and when moving away from the interface ( $\kappa x \gg 1$ ).

### 8.8.2 Finding the Dispersion Equation from the Asymptotic Flux

It is shown that the dispersion equation can also be found directly by integrating the integro-differential equation (Tait 1964, p 28). Starting again from the $1 D$ transport equation:

$$
\mu \frac{\partial \Phi(x, \mu)}{\partial x}+\Sigma_{t} \Phi(x, \mu)=\frac{c \Sigma_{t}}{2} \int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}=\frac{c \Sigma_{t}}{2} \Phi(x)
$$

Multiplying each term by: $e^{\frac{\Sigma_{t}}{\mu} x} / \mu$, we find:

$$
\frac{\partial\left[e^{\frac{\Sigma_{t}}{\mu} x} \Phi(x, \mu)\right]}{\partial x}=\frac{c \Sigma_{t}}{2 \mu} e^{\frac{\Sigma_{t}}{\mu} x} \Phi(x)
$$

For $\mu>0$, this equation is integrated over $x$ over the domain $]-\infty, x]$ to obtain:

$$
e^{\frac{\Sigma_{t}}{\mu} x} \Phi(x, \mu)=\frac{c \Sigma_{t}}{2 \mu} \int_{-\infty}^{x} e^{\frac{\Sigma_{t}}{\mu} x^{\prime}} \Phi\left(x^{\prime}\right) d x^{\prime}
$$

Similar, for $\mu<0$, the integration is over $[x,+\infty[$ :

$$
-e^{\frac{\Sigma_{t}}{\mu} x} \Phi(x, \mu)=\frac{c \Sigma_{t}}{2 \mu} \int_{c v}^{+\infty} e^{\frac{\Sigma_{t}}{\mu} x^{\prime}} \Phi\left(x^{\prime}\right) d x^{\prime}
$$

The integrated flux $\Phi(x)$ is then calculated using these two expressions:

$$
\begin{aligned}
\Phi(x) & =\int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime} \\
& =\int_{0}^{1} e^{-\frac{\Sigma_{t}}{\mu} x} \frac{c \Sigma_{t}}{2 \mu^{\prime}} \int_{-\infty}^{x} e^{\frac{\Sigma_{t}}{\mu^{\prime}}} \Phi\left(x^{\prime}\right) d x^{\prime} d \mu^{\prime}-\int_{-1}^{0} e^{-\frac{\Sigma_{t}}{\mu} x} \frac{c \Sigma_{t}}{2 \mu^{\prime}} \int_{c v}^{+\infty} e^{\frac{\Sigma_{t}}{\mu} x^{\prime}} \Phi\left(x^{\prime}\right) d x^{\prime} d \mu^{\prime} \\
& =\frac{c \Sigma_{t}}{2} \int_{0}^{1} \frac{1}{\mu^{\prime}} \int_{-\infty}^{+\infty} e^{\frac{\Sigma_{t}}{\mu}\left|x-x^{\prime}\right|} \Phi\left(x^{\prime}\right) d x^{\prime} d \mu^{\prime}=\frac{c \Sigma_{t}}{2} \int_{-\infty}^{+\infty} E_{1}\left(\Sigma_{t}\left|x-x^{\prime}\right|\right) \Phi\left(x^{\prime}\right) d x^{\prime}
\end{aligned}
$$

by using the integral of the exponential function: $E_{1}(x)=\int_{1}^{+\infty} \frac{1}{t} e^{-t x} d t$. The flux in the integral is then replaced by its Taylor expansion:

$$
\Phi\left(x^{\prime}\right)=\Phi(x)+\left.\sum_{n=1}^{+\infty} \frac{1}{n!} \frac{d^{n} \Phi}{d x^{n}}\right|_{x}\left(x^{\prime}-x\right)^{n}
$$

$$
\text { to give : } \begin{aligned}
& \int_{-\infty}^{+\infty} E_{1}\left(\Sigma_{t}\left|x-x^{\prime}\right|\right)\left(x^{\prime}-x\right) d x^{\prime} \\
= & \int_{0}^{+\infty} \int_{1}^{+\infty} \frac{1}{t} e^{-t \Sigma_{t}\left(x^{\prime}-x\right)}\left(x^{\prime}-x\right) d t d x^{\prime}+\int_{-\infty}^{0} \int_{1}^{+\infty} \frac{1}{t} e^{-t \Sigma_{t}\left(x-x^{\prime}\right)}\left(x^{\prime}-x\right) d t d x^{\prime} \\
= & \int_{1}^{+\infty} \frac{1}{t^{3} \Sigma_{t}^{2}} \int_{0}^{+\infty} e^{-y} y d y-\int_{1}^{+\infty} \frac{1}{t^{3} \Sigma_{t}^{2}} \int_{0}^{+\infty} e^{-y} y d y=0
\end{aligned}
$$

The $d \Phi / d x$ term is zero as well as all the odd derivative terms. Regarding the even terms:

$$
\int_{-\infty}^{+\infty} E_{1}\left(\Sigma_{t}\left|x-x^{\prime}\right|\right) \frac{1}{(2 k)!}\left(x^{\prime}-x\right)^{2 k} d x^{\prime}=2 \int_{1}^{+\infty} \frac{1}{t^{2 k+2} \Sigma_{t}^{2 k+1}} \underbrace{\left(\int_{0}^{+\infty} e^{-y} y^{2 k} d y\right)}_{\Gamma(2 k+1)=(2 k)!} d t=\frac{2}{(2 k+1) \Sigma_{t}^{2 k+1}}
$$

which allows us to write:

$$
\Phi(x)=c\left(\Phi(x)+\frac{1}{3 \Sigma_{t}^{2}} \frac{d^{2} \Phi(x)}{d x^{2}}+\frac{1}{5 \Sigma_{t}^{4}} \frac{d^{4} \Phi(x)}{d x^{4}}+\frac{1}{7 \Sigma_{t}^{6}} \frac{d^{6} \Phi(x)}{d x^{6}}+\cdots\right)
$$

In a non-multiplicative medium where the flux would satisfy: $d^{2} \Phi(x) / d x^{2}=$ $\kappa^{2} \Phi(x)$, the equation in $\mathrm{c}, \kappa$ and $\Sigma_{t}$ is obtained:

$$
1=c\left(1+\frac{1}{3 \Sigma_{t}^{2}} \kappa^{2}+\frac{1}{5 \Sigma_{t}^{4}} \kappa^{4}+\frac{1}{7 \Sigma_{t}^{6}} \kappa^{6}+\cdots\right)
$$

which will be expressed in the form:

$$
\frac{\kappa}{c \Sigma_{t}}=\left(\frac{\kappa}{\Sigma_{t}}+\frac{\kappa^{3}}{3 \Sigma_{t}^{3}}+\frac{\kappa^{5}}{5 \Sigma_{t}^{5}}+\frac{\kappa^{7}}{7 \Sigma_{t}^{7}}+\cdots\right)
$$

so as to obtain on the right-hand side the limited power series of $\tanh ^{-1}\left(\kappa / \Sigma_{t}\right)$. The previous equation can hence be rewritten in the known form of the dispersion equation, which indeed corresponds to a closure relation for the exponential attenuation coefficient of the asymptotic flux.

$$
\frac{\kappa}{\Sigma_{t}}=\tanh \left(\frac{\kappa}{c \Sigma_{t}}\right)
$$

### 8.8.3 Critical Absorption Limiting the Asymptotic Solution

To understand the importance of absorption with respect to the resulting asymptotic solution, the simple case of an infinite medium without source terms, a constant isotropic scattering cross section and absorption cross section with a $1 / v$ shape, will be considered here. The kernel for scattering is separable as seen previously in thermalization, and the scattering cross section obeys the detailed balance principle (Neutron thermalization $1962 \mathrm{pRF}-17$ ):
$\Sigma_{s}\left(E^{\prime} \rightarrow E, \mu_{0}\right)=\frac{\Sigma_{s, 0}}{2} m(E)$ where $m(E)$ is the maxwellian distribution with energy $k T$

For the purpose of coherence, the usual coefficient of 2 (arising with expansions in Legendre polynomials) was retained. From now on, the reduced energy $y=E /(k T)$ will be used. With these assumptions, the total cross section is written:

$$
\Sigma_{t}(y)=\frac{\Sigma_{s, 0}}{2}(1+\gamma \sqrt{y}) \quad \text { and } \quad m(y)=y e^{-y}
$$

The Boltzmann equation is given:

$$
\mu \frac{\partial \Phi(x, y, \mu)}{\partial x}+\Sigma_{t}(y) \Phi(x, y, \mu)=\int_{0}^{+\infty} d y^{\prime} \int_{-1}^{+1} \Sigma_{s}\left(y^{\prime} \rightarrow y, \mu^{\prime}\right) \Phi\left(x, y^{\prime}, \mu^{\prime}\right) d \mu^{\prime}
$$

With the flux expressed in the form $\Phi(x, y, \mu)=e^{-\kappa x} \Phi(y, \mu)$, we find:

$$
\mu \kappa e^{-\kappa x} \frac{\partial \Phi(y, \mu)}{\partial x}+\Sigma_{t}(y) e^{-\kappa x} \Phi(y, \mu)=\int_{0}^{+\infty} d y^{\prime} \int_{-1}^{+1} \frac{\Sigma_{s, 0}}{2} m(y) e^{-\kappa x} \Phi\left(y^{\prime}, \mu^{\prime}\right) d \mu^{\prime}
$$

Hence after simplifying:

$$
\Phi(y, \mu)=\frac{m(y)}{\left[\mu \kappa+\frac{\Sigma_{s, 0}}{2}(1+\gamma \sqrt{y})\right]} \int_{0}^{+\infty} d y^{\prime} \int_{-1}^{+1} \frac{\Sigma_{s, 0}}{2} \Phi\left(y^{\prime}, \mu^{\prime}\right) d \mu^{\prime}
$$

Setting $K=2 \kappa / \Sigma_{s, 0}$ and integrating the previous equation over $\mu \in[-1,+1]$ and over the reduced energy $y$, we find a particular form of the dispersion equation:

Dispersion equation with a $1 / v$ absorption:

$$
\begin{equation*}
K=\int_{0}^{+\infty} \ln \left(\frac{1+\gamma \sqrt{y}+K}{1+\gamma \sqrt{y}-K}\right) m(y) d y=\int_{0}^{+\infty} \ln \left(1+2 \frac{\sqrt{y}}{\gamma}\right) m(y) d y \tag{8.63}
\end{equation*}
$$

The integral term on the right-hand side is an increasing function with respect to $K$ and decreasing with respect to $\gamma$, varying from $\ln (1+2 K)$ for $\gamma=0$, to 0 when $\gamma \rightarrow+\infty$. When $K=1$, there exists a critical value $\gamma_{c}$, such that:

$$
1=\int_{0}^{+\infty} \ln \left(1+2 \frac{\sqrt{y}}{\gamma_{c}}\right) m(y) d y
$$

If $\gamma>\gamma_{c}$, the right-hand side term of the dispersion equation is always less than $K \in[0,1]$. There is then no solution to the eigenvalue problem. $\gamma_{c}$ is of the order of 1 , which corresponds approximately to the case where the absorption is of the same
order of magnitude as diffusion with energy $k T$. It is quite easy and intuitive to imagine that a too big absorption would impair the setting up of an asymptotic diffusion regime. If the neutrons have a $50 \%$ chance of being absorbed, they cannot be scattered anymore and the thermalization phase is impossible. This result has been shown for a simple example but remains valid in the case of more physical cross sections: the flux will not satisfy a diffusion equation in case of too strong absorption. This fundamental assumption of diffusion, which will be discussed again in Chap. 10, is however largely absent in physics calculations of industrial reactors.

### 8.8.4 Definition of a Diffusion Coefficient from the Transport Equation

We have seen previously that the monokinetic transport equation allows for solutions of the form:

$$
\Phi(\mathrm{x}, \mu)=\Phi_{\nu}(\mu) e^{ \pm \frac{\mathrm{x}}{\nu}}=\Phi_{k}(\mu) e^{ \pm \mathrm{k} x}
$$

in Case's notations. These solutions satisfy a Helmholtz equation of the form:

$$
\Delta \Phi-\frac{1}{\nu^{2}} \Phi=\Delta \Phi-k^{2} \Phi=0
$$

This diffusion equation hence has to be able to be applied in a sufficiently large medium such that we can assume being far from boundaries or sources that cause transients. In a fissile homogeneous medium without external sources, the Boltzmann equation is written:

$$
\begin{aligned}
\vec{\Omega} . \overrightarrow{g r a d} \Phi(\vec{r}, E, \vec{\Omega})+\Sigma_{t}(E) \Phi(\vec{r}, E, \vec{\Omega})= & \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{S}\left(E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega},\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right) \\
& +\frac{\chi(E)}{4 \pi} \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \int_{4 \pi} d \vec{\Omega}^{\prime} \quad \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

Applying a $3 D$ spatial Fourier transform, justified by the homogeneous properties of the medium, and invariant by translation:

$$
\phi(\vec{k}, E, \vec{\Omega})=\int_{\vec{r}} d \vec{r} \quad e^{i \vec{k} \cdot \vec{r}} \Phi(\vec{r}, E, \vec{\Omega})
$$

The transport equation can then be rewritten in terms of the Fourier transform $\phi$ :

$$
\begin{aligned}
\left(\Sigma_{t}(E)-i \vec{k} . \vec{\Omega}\right) \phi(\vec{k}, E, \vec{\Omega})= & \int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \phi\left(\vec{k}, E^{\prime}, \vec{\Omega}^{\prime}\right) \\
& +\frac{\chi(E)}{4 \pi} \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right)
\end{aligned}
$$

This Fredholm integral equation has solutions only for some discrete values of the vector $\vec{k}$. By integrating over all directions $\vec{\Omega}$, we find:

$$
\begin{align*}
\Sigma_{t}(E) \phi(\vec{k}, E)-i \vec{k} \cdot \vec{J}(\vec{k}, E)= & \int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(\vec{k}, E^{\prime}\right) \\
& +\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right) \tag{8.64}
\end{align*}
$$

We introduce the Fourier transform of the current:

$$
\vec{J}(\vec{k}, E)=\int_{4 \pi} d \vec{\Omega} \vec{\Omega} \cdot \phi\left(\vec{k}, E^{\prime}, \vec{\Omega}\right)
$$

and the Fourier transform of the flux, integrated over angle:

$$
\phi(\vec{k}, E)=\int_{4 \pi} d \vec{\Omega} \phi\left(\vec{k}, E^{\prime}, \vec{\Omega}\right)
$$

as well as the scattering cross section:

$$
\Sigma_{s}\left(E^{\prime} \rightarrow E\right)=\int_{4 \pi} d \vec{\Omega} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right)
$$

Let us assume a linearly anisotropic collision. By expanding the scattering cross section in terms of the cosine of the collision angle (the scalar product of the angular direction before and after the collision $\mu \equiv \vec{\Omega}^{\prime} \cdot \vec{\Omega}$ ), using Legendre polynomials up to the first order term, we find:

$$
\Sigma_{s}\left(E^{\prime} \rightarrow E, \vec{\Omega}^{\prime} \cdot \vec{\Omega}\right)=\frac{\Sigma_{s, 0}\left(E^{\prime} \rightarrow E\right)}{4 \pi}+\frac{3 \Sigma_{s, 1}\left(E^{\prime} \rightarrow E\right) \vec{\Omega}^{\prime} \cdot \vec{\Omega}}{4 \pi}
$$

with the isotropic part being given by:

$$
\Sigma_{s, 0}\left(E^{\prime} \rightarrow E\right)=\int_{\mu} d \mu \quad \Sigma_{s}\left(E^{\prime} \rightarrow E, \mu\right)
$$

and the first moment by:

$$
\Sigma_{s, 1}\left(E^{\prime} \rightarrow E\right)=\int_{\mu} d \mu \mu \cdot \Sigma_{s}\left(E^{\prime} \rightarrow E, \mu\right)
$$

With these notations, the equation in terms of the Fourier transform of the flux can be rewritten:

$$
\begin{aligned}
\phi(\vec{k}, E, \vec{\Omega}) & =\frac{1}{4 \pi} \frac{1}{\Sigma_{t}(E)-i \vec{k} \cdot \vec{\Omega}}\left[\int_{0}^{\infty} d E^{\prime} \Sigma_{s, 0}\left(E^{\prime} \rightarrow E\right) \phi\left(\vec{k}, E^{\prime}\right)\right. \\
& \left.+3 \vec{\Omega} \int_{0}^{\infty} d E^{\prime} \Sigma_{s, 1}\left(E^{\prime} \rightarrow E\right) \vec{J}\left(\vec{k}, E^{\prime}\right)+\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \varphi\left(\vec{k}, E^{\prime}\right)\right]
\end{aligned}
$$

Integrating this last equation over all directions $\vec{\Omega}$, we obtain:

$$
\begin{align*}
\phi(\vec{k}, E)= & \int_{4 \pi} d \vec{\Omega} \phi(\vec{k}, E, \vec{\Omega})=\frac{\tan ^{-1}\left(\frac{\|\vec{k}\|}{\Sigma_{t}(E)}\right)}{\|\vec{k}\|} \\
& {\left[\int_{0}^{\infty} d E^{\prime} \Sigma_{s, 0}\left(E^{\prime} \rightarrow E\right) \phi\left(\vec{k}, E^{\prime}\right)+\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right)\right] } \\
& +\frac{i}{\|\vec{k}\|}\left(1-\frac{\Sigma_{t}(E)}{\|\vec{k}\|} \tan ^{-1}\left(\frac{\|\vec{k}\|}{\Sigma_{t}(E)}\right)\right) \times 3 \vec{\Omega} \int_{0}^{\infty} d E^{\prime} \Sigma_{s, 1}\left(E^{\prime} \rightarrow E\right) \vec{J}\left(\vec{k}, E^{\prime}\right) \tag{8.65}
\end{align*}
$$

To simplify notation, we define $k \equiv\|\vec{k}\|$ and the scalar function below is introduced:

$$
J(\vec{k}, E) \equiv \frac{\vec{k} \cdot \vec{J}(\vec{k}, E)}{k}=\frac{1}{k} \int_{4 \pi} d \vec{\Omega} \vec{k} \cdot \vec{\Omega} \cdot \phi(\vec{k}, E, \vec{\Omega})
$$

From Eq. 8.64, it can be deduced that:

$$
\begin{equation*}
\vec{k} \cdot \vec{J}(\vec{k}, E)=\frac{\Sigma_{t}(E) \phi(\vec{k}, E)-\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(\vec{k}, E^{\prime}\right)-\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right)}{i} \tag{8.66}
\end{equation*}
$$

which is substituted in, in Eq. 8.65, to yield:

$$
\begin{align*}
\phi(\vec{k}, E)= & \int_{4 \pi} d \vec{\Omega} \phi(\vec{k}, E, \vec{\Omega}) \\
& =\frac{\operatorname{Arctan}\left(\frac{\|\vec{k}\|}{\Sigma_{t}(E)}\right)}{\|\vec{k}\|}\left[\int_{0}^{\infty} d E^{\prime} \Sigma_{s, 0}\left(E^{\prime} \rightarrow E\right) \phi\left(\vec{k}, E^{\prime}\right)\right. \\
+ & \left.\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right)\right] \\
+ & \frac{i}{\|\vec{k}\|}\left(1-\frac{\Sigma_{t}(E)}{\|\vec{k}\|} \operatorname{Arctan}\left(\frac{\|\vec{k}\|}{\Sigma_{t}(E)}\right)\right) \\
& \times 3 \vec{\Omega} \int_{0}^{\infty} d E^{\prime} \Sigma_{s, 1}\left(E^{\prime} \rightarrow E\right) \vec{J}\left(\vec{k}, E^{\prime}\right) \tag{8.67}
\end{align*}
$$

Here again, this equation has solutions only for some complex eigenvalues of the parameter $k$, which can only vary within the definition of the unique function Arctan $\left(k / \Sigma_{t}(E)\right) / k$ in the complex plane, already illustrated in Fig. 8.30. This plane is cut by the complex straight half-lines $\left\lfloor+i \Sigma_{t, \text { min }},+i \infty\lfloor\right.$ and $\left.\rfloor-i \infty,-i \Sigma_{t, \text { min }}\right\rfloor, \Sigma_{t, \text { min }}$ being the minimum of the total cross section. This is called "Corngold's hypothesis", after the work of Noel Corngold. ${ }^{60}$ Denoting the eventually complex eigenvalue of smallest magnitude (compared to the other eigenvalues) by $k_{0}$ and the associated fundamental flux by $\phi\left(k_{0}, E\right)$, Eq. 8.66 is given by (Fig. 8.31):

$$
\begin{align*}
J\left(k_{0}, E\right)= & \frac{i}{k_{0}}\left(-\Sigma_{t}(E) \phi(\vec{k}, E)+\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(\vec{k}, E^{\prime}\right)\right. \\
& \left.+\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right)\right) \tag{8.68}
\end{align*}
$$

[^181]A diffusion coefficient can then be introduced:

$$
D\left(k_{0}, E\right) \equiv-\frac{i}{k_{0}} \frac{J\left(k_{0}, E\right)}{\phi\left(k_{0}, E\right)}
$$

Which, when substituted in Eq. 8.68, allows us to write:

$$
\begin{aligned}
\left(\Sigma_{t}(E)+D\left(k_{0}, E\right) k_{0}^{2}\right) \phi\left(k_{0}, E\right) & =\int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \phi\left(k_{0}, E^{\prime}\right) \\
& +\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \varphi\left(k_{0}, E^{\prime}\right)
\end{aligned}
$$

Through the inverse Fourier transform of the previous equation, the spatial flux spectrum:

$$
\Phi(\vec{r}, E)=e^{-i \overrightarrow{k_{0}} \cdot \vec{r}} \phi\left(k_{0}, E\right)
$$

is the solution of the diffusion equation:

$$
\begin{aligned}
-D\left(k_{0}, E\right) \Delta \Phi(\vec{r}, E)+\Sigma_{t}(E) \Phi(\vec{r}, E)= & \int_{0}^{\infty} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}\right) \\
& +\chi(E) \int_{0}^{\infty} d E^{\prime} \nu \Sigma_{f}\left(E^{\prime}\right) \Phi\left(\vec{r}, E^{\prime}\right)
\end{aligned}
$$


(Courtesy Corngold)

The fundamental flux and the diffusion coefficient can be evaluated by considering Eq. 8.67. By imposing a normalization, for one neutron produced, such as:

$$
\int_{0}^{\infty} d E \nu \Sigma_{f}(E) \phi(\vec{k}, E)=1
$$

and using the conventional notations:

$$
\alpha(k, E)=\frac{\operatorname{Arctan}\left(\frac{k}{\Sigma_{t}(E)}\right)}{k} \quad \text { and } \quad \beta(k, E)=\frac{1}{k^{2}}\left(1-\frac{\Sigma_{t}(E)}{k} \operatorname{Arctan}\left(\frac{k}{\Sigma_{t}(E)}\right)\right)
$$

Equation 8.67 can be rewritten in the form:

$$
\begin{aligned}
\phi(k, E)= & \alpha(k, E)\left[\int_{0}^{\infty} d E^{\prime} \Sigma_{s, 0}\left(E^{\prime} \rightarrow E\right) \phi\left(k, E^{\prime}\right)+\chi(E)\right] \\
& -\beta(k, E) \times 3 \int_{0}^{\infty} d E^{\prime} \Sigma_{s, 1}\left(E^{\prime} \rightarrow E\right) \quad\left(\int_{0}^{\infty} d E^{\prime \prime} \quad \Sigma_{s}\left(E^{\prime \prime} \rightarrow E^{\prime}\right) \phi\left(\vec{k}, E^{\prime \prime}\right)\right. \\
& \left.+\chi\left(E^{\prime}\right)-\Sigma_{t}\left(E^{\prime}\right) \phi\left(\vec{k}, E^{\prime}\right)\right)
\end{aligned}
$$

The solution $\varphi(k, E)$ of the previous equation is the solution to Eq. 8.67 as well if it satisfies the normalization condition; therefore, $k$ is the root of the function:

$$
\int_{0}^{\infty} d E \nu \Sigma_{f}(E) \phi(\vec{k}, E)-1=0
$$

In a supercritical medium, $k$ is real while in a subcritical medium, $k$ is purely imaginary. The previous theory can be generalized without any difficulty for multigroup. For the usual two energy groups in diffusion theory (cutoff at 0.625 eV ), this model provides, for a conventional fuel, a rapid diffusion coefficient of the order of 1.3 cm and a thermal diffusion coefficient of about 0.4 cm in the $\mathrm{B}_{0}$ approximation (isotropic scattering cross section). Taking into account a $B_{1}$ anisotropy for the scattering cross section tends to increase the rapid diffusion coefficients to values close to 1.45 cm .

### 8.9 The 3D Transport Equations

The $1 D$ case certainly remains very interesting, at least for an analytical treatment; however most realistic cases are three-dimensional.

In Cartesian geometry, the steady-state transport equation is written:

$$
\begin{aligned}
& \mu \frac{\partial \Phi(x, y, z, \vec{\Omega})}{\partial x}+\eta \frac{\partial \Phi(x, y, z, \vec{\Omega})}{\partial y}+\xi \frac{\partial \Phi(x, y, z, \vec{\Omega})}{\partial z}+\Sigma_{t} \Phi(x, y, z, \vec{\Omega}) \\
& \quad=S(x, y, z, \vec{\Omega})
\end{aligned}
$$

with the usual notations: $\mu \equiv \vec{\Omega} \cdot \overrightarrow{u_{x}}, \eta \equiv \vec{\Omega} \cdot \overrightarrow{u_{y}}$ and $\xi \equiv \vec{\Omega} \cdot \overrightarrow{u_{z}}$, with $S(x, y, z, \vec{\Omega})$ representing the fission or scattering source of neutrons. The vectors $\vec{u}$ are the unit vectors along each axis. The three cosines are related through the expression:

$$
\mu^{2}+\eta^{2}+\xi^{2}=1
$$

In Cartesian geometry, the current is given by:

$$
\vec{J}=\left(\begin{array}{l}
J_{x} \\
J_{y} \\
J_{z}
\end{array}\right)=\left(\begin{array}{c}
-\frac{1}{3 \Sigma_{t}} \frac{\partial \Phi}{\partial x} \\
-\frac{1}{3 \Sigma_{t}} \frac{\partial \Phi}{\partial y} \\
-\frac{1}{3 \Sigma_{t}} \frac{\partial \Phi}{\partial z}
\end{array}\right)
$$

In cylindrical geometry (Fig. 8.33), the equation is given by:

$$
\begin{aligned}
& \frac{\mu}{r} \frac{\partial(r \Phi(r, \theta, z, \vec{\Omega}))}{\partial r}+\frac{\eta}{r} \frac{\partial \Phi(r, \theta, z, \vec{\Omega})}{\partial \theta}+\xi \frac{\partial \Phi(r, \theta, z, \vec{\Omega})}{\partial z}-\frac{1}{r} \frac{\partial(\eta \Phi(r, \theta, z, \vec{\Omega}))}{\partial \omega} \\
& +\Sigma_{t} \Phi(r, \theta, z, \vec{\Omega})=S(r, \theta, z, \vec{\Omega})
\end{aligned}
$$



Fig. 8.33 Cylindrical coordinates used in the cylindrical Boltzmann equation

With $\mu \equiv \vec{\Omega} \cdot \overrightarrow{u_{r}}=\sqrt{\left(1-\xi^{2}\right)} \cos \omega, \eta \equiv \vec{\Omega} \cdot \overrightarrow{u_{\theta}}=\sqrt{\left(1-\xi^{2}\right)} \sin \omega, \xi \equiv \vec{\Omega} \cdot \overrightarrow{u_{z}}$.
The current is written:

$$
\vec{J}=\left(\begin{array}{l}
J_{r} \\
J_{\theta} \\
J_{z}
\end{array}\right)=\left(\begin{array}{c}
-\frac{1}{3 \Sigma_{t}} \frac{\partial \Phi}{\partial r} \\
-\frac{1}{3 \Sigma_{t} r} \frac{\partial \Phi}{\partial \theta} \\
-\frac{1}{3 \Sigma_{t}} \frac{\partial \Phi}{\partial z}
\end{array}\right)
$$

and:

$$
\Phi(r, \theta, \varphi, \vec{\Omega})=\Phi(r, \theta, \varphi, \mu, \omega)=\Phi(r, \theta, \varphi)+3 \mu J_{r}+3 \eta J_{\theta}+3 \xi J_{z}
$$

In spherical coordinates-recall that we had already seen the coordinate representation in Fig. 8.32, the Boltzmann equation is given by:

$$
\begin{aligned}
& \frac{\mu}{r^{2}} \frac{\partial\left(r^{2} \Phi(r, \theta, \varphi, \vec{\Omega})\right)}{\partial r}+\frac{\eta}{r \sin \theta} \frac{\partial \Phi(r, \theta, \varphi, \vec{\Omega})}{\partial \theta}+\frac{\xi}{r \sin \theta} \frac{\partial(\sin \theta \Phi(r, \theta, \varphi, \vec{\Omega}))}{\partial \varphi} \\
& \quad+\frac{1}{r} \frac{\partial\left(\left(1-\mu^{2}\right) \Phi(r, \theta, \varphi, \vec{\Omega})\right)}{\partial \mu}-\frac{\cot \theta}{r} \frac{\partial(\xi \Phi(r, \theta, \varphi, \vec{\Omega}))}{\partial \mu}+\Sigma_{t} \Phi(r, \theta, z, \vec{\Omega}) \\
& =S(r, \theta, z, \vec{\Omega})
\end{aligned}
$$

with $\eta=\sqrt{\left(1-\mu^{2}\right)} \cos \omega, \xi=\sqrt{\left(1-\mu^{2}\right)} \sin \omega$.
The current is written:

$$
\vec{J}=\left(\begin{array}{c}
J_{r} \\
J_{\theta} \\
J_{\phi}
\end{array}\right)=\left(\begin{array}{c}
-\frac{1}{3 \Sigma_{t}} \frac{\partial \Phi}{\partial r} \\
-\frac{1}{3 \Sigma_{t} r \sin \theta} \frac{\partial \Phi}{\partial \theta} \\
-\frac{1}{3 \Sigma_{t} r} \frac{\partial \Phi}{\partial \phi}
\end{array}\right)
$$

It should be noted that:

$$
\Phi(r, \theta, \varphi, \vec{\Omega})=\Phi(r, \theta, \varphi, \mu, \omega)=\Phi(r, \theta, \varphi)+3 \mu J_{r}+3 \eta J_{\theta}+3 \xi J_{\phi}
$$

One should be careful ${ }^{61}$ of the fact that the angle $\theta$ in spherical coordinates is the colatitude and does not correspond to the usual definition of this angle in cylindrical geometry. Here, it was preferred to use the colatitude as in (Lewis and Miller 1993, p32).

During transients, the term $\frac{1}{v} \frac{\partial \Phi(t)}{\partial t}$ is simply added to the previous equations.

[^182]
## Chapter 9 <br> Computational Neutron Transport Methods

The Boltzmann equation is difficult to solve in practical cases and only a few textbook cases have an analytical solution. Thus, myriad numerical methods have been set up for its resolution and will be discussed briefly in this chapter. Beginning in 1943, with the Manhattan Project for the design of the atomic bomb in the United States, numerical methods specific to the transport equations have been schemed for the first computers. The Monte Carlo method is different from the other methods since it does not solve the Boltzmann equation as such but simulates an analogous path of neutrons in matter.

Gerald Pomraning, in Reactor Physics, vol. 1, pp. 207-257 (1966), Richard Sanchez and N.J. McCormick, in Nuclear Science and Engineering, vol. 80, pp. 481-535 (1982).

### 9.1 Discrete Ordinates Method $\boldsymbol{S}_{\boldsymbol{n}}$

(Duderstadt and Martin 1979; Bussac and Reuss 1985; Lewis and Miller 1993; Clark and Hansen 1964, p. 204; Baur 1985, p. 220; Bellman et al. 1969, p. 129; Stacey 2001, p. 353; Stamm'ler and Abbate 1983, p. 191; Contrôle de la criticalité 1961, p. 83).

Bengt G. Carlson ${ }^{1,2,3}$ proposed an approach for dealing with the angular part of the transport equation. It consists in substituting the integro-differential equation continuous with the angle by a system of differential equations in a finite number of directions $\vec{\Omega}_{n}$. Thus, the angular flux is represented by a set of discrete values called the discrete ordinates (Fig. 9.1):


Bengt G. Carlson (1916-2007), founder of the discrete ordinates method (The Marguet collection, photograph unknown)

Since Gauss, it is well-known that some wisely-chosen quadratures lead to efficient integration of the function $\Phi(\vec{\Omega})$ :

[^183]Fig. 9.1 Discrete ordinates method


$$
\int_{4 \pi} \Phi(\vec{\Omega}) d \vec{\Omega}=\sum_{i=1}^{N} \varpi_{i} \Phi\left(\vec{\Omega}_{i}\right)
$$

where $\varpi_{i=1, N}$ are the weights of the chosen quadrature and $N$ the number of Gauss points of the quadrature (Grandini 1986, p. 189; Bathe 1982, p. 274). With this angular discretization, the Boltzmann equation is equivalent to a system of $N$ coupled differential equations:

$$
\begin{aligned}
& \frac{1}{v} \frac{\partial \Phi\left(\vec{r}, E, \vec{\Omega}_{i}, t\right)}{\partial t}+\vec{\Omega}_{i} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, E, \vec{\Omega}, t)+\Sigma_{t}(\vec{r}, E, \vec{\Omega}, t) \Phi(\vec{r}, E, \vec{\Omega}, t) \\
& \quad=S(\vec{r}, E, \vec{\Omega}, t)+\sum_{j=1}^{N} \varpi_{j} \int_{0}^{\infty} d E^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega}_{j} \rightarrow \vec{\Omega}_{i}, t\right) \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}_{j}, t\right)
\end{aligned}
$$

In this equation, there are as many $\Phi\left(\vec{r}, E, \vec{\Omega}_{i}, t\right)$ terms as the number of independent angles $\Phi(\vec{r}, E, t) \equiv \Phi(\vec{r}, E, \vec{\Omega}, t)$ The risk of this approach, called the $S_{n}$ method, is the fact that only the spatial distribution of these functions $\Phi(\vec{r}, E, t)$ are known, i.e. only for some chosen directions. This effect is called the ray effect ${ }^{4}$ and can be observed readily in the case of a non-scattering medium. Indeed, for instance, the flux due to a point source is strictly zero for directions that do not belong to the quadrature, which is not consistent with a constant-valued flux as expected for a given distance from the source (Fig. 9.2).

[^184]

Fig. 9.2 The ray effect: an isotropic source is placed in a square of sides $0.2 \times 0.2 \mathrm{~cm}$ and emits neutrons in a square material of sides 10 cm and total cross section $0.1 \mathrm{~cm}^{-1}$. The calculation was carried out with an S8 quadrature with ten directions per quadrant of the unit sphere. The expected theoretical result is a uniformly-decreasing distribution from the source. The ray effect is clearly visible around the directions of the quadrature, which are the only zones with a non-zero flux (iconography: Emiliano Masiello from his work on the IDT code, $C E A, 2009)$

If the angular discretization is chosen randomly and does not conserve the physics of the phenomena, some unusual flux behavior can be completely overlooked (e.g. anisotropy). However, the ray effect is less dominant in a reactor where the media are highly scattering and the sources are well distributed (in fact, the ray effect has been discovered more than 15 years after the method was conceived). For the directions that are not covered, several interpolation methods can be employed. In this case, it can be intuitively understood that an isotropic flux is particularly adapted for such approaches since a limited sampling is sufficient to obtain the complete distribution by interpolation. The discrete ordinates method is an alternative to flux expansion on a basis of functions (Legendre ${ }^{5}$ polynomials or spherical harmonics for

[^185]instance) which will be discussed further on. In the case of a $l D$ problem where the flux depends only on the variable $x$ and $\mu=\cos \theta$, the Gauss quadrature is optimum for integration. It can be shown that this particular quadrature (the Gauss points are the roots of the Legendre polynomials) is rigorously equivalent to a $P_{n-1}$ approximation, even though the flux moments are not calculated as in the $P_{n}$ method which will be seen later on. The scattering operator can be expanded and projected on a spherical function basis at order $n$ (which should not be confused with the total number of points in the quadrature $N$ ), in a time-independent case (to simplify notations, but it can also be extended to the transient case), and for one energy group (once more, the extension to multi-group is also possible):
\[

$$
\begin{aligned}
& \vec{\Omega}_{i} \cdot \overrightarrow{\operatorname{grad}} \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)+\Sigma_{t}\left(\vec{r}, \vec{\Omega}_{i}\right) \Phi\left(\vec{r}, \vec{\Omega}_{i}\right) \\
& \quad=S\left(\vec{r}, \vec{\Omega}_{i}\right)+\sum_{l=1}^{N} \sum_{m=-l}^{m=+l} Y_{l}^{m}\left(\vec{\Omega}_{i}\right) \Sigma_{S, l}(\vec{r}) \Phi_{l}^{m}(\vec{r}) \quad \text { for } i=1, N
\end{aligned}
$$
\]

where: $\Phi_{l}^{m}(\vec{r})=\int_{4 \pi} d \vec{\Omega} \overline{Y_{l}^{m}\left(\vec{\Omega}_{i}\right)} \Phi(\vec{r}, \vec{\Omega})=\sum_{I=1}^{N} \varpi_{i} \overline{Y_{l}^{m}\left(\vec{\Omega}_{i}\right)} \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)$
Thus, a coupled system of linear equations with respect to the angle is obtained and expressed in matrix form as:

$$
\begin{equation*}
\left(\vec{\Omega} \cdot \overrightarrow{g r a d}+\Sigma_{t}\right)[\Phi]=R[\Phi]+S \tag{9.1}
\end{equation*}
$$

where:

- [ $\Phi]$ is the column vector of the flux components per direction of the discrete ordinates, which are themselves expanded as flux of the angular quadrature,
- $R$ is the slowing-down operator matrix,
- $S$ the source matrix,
- $\left(\vec{\Omega} \cdot \overrightarrow{g r a d}+\Sigma_{t}\right)$ the transport matrix.

Equation (9.1) must be discretized spatially, for instance using the finite difference method or the nodal method by assuming an intra-nodal flux shape, and also discretized in energy using a multi-group approach. If scattering is isotropic, it is simplified as:

$$
\vec{\Omega}_{i} \cdot \overrightarrow{g r a d} \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)+\Sigma_{t}\left(\vec{r}, \vec{\Omega}_{i}\right) \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)=S\left(\vec{r}, \vec{\Omega}_{i}\right)+\frac{\Sigma_{S}(\vec{r})}{4 \pi} \sum_{i=1}^{N} \varpi_{i} \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)
$$

This is logical since $\Phi(\vec{r})=\sum_{i=1}^{N} \varpi_{i} \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)$ and the number of neutrons scattered isotropically in any direction is given as $\Sigma_{S}(\vec{r}) \Phi(\vec{r}) / 4 \pi$.

The current is expressed as follows:

$$
\vec{J}(\vec{r})=\sum_{i=1}^{N} \varpi_{i} \vec{\Omega}_{i} \Phi\left(\vec{r}, \vec{\Omega}_{i}\right)
$$

In the case of a one-dimensional geometry (plane or sphere), an angular discretization with Straight lines ${ }^{6}$ (thus the term $S_{n}$ or trapezoidal quadrature) was used such that the flux was reconstructed linearly between two values of the angle cosine:

$$
\Phi(x, \mu)=\frac{\mu-\mu_{i-1}}{\mu_{i}-\mu_{i-1}} \Phi\left(x, \mu_{i}\right)+\frac{\mu_{i}-\mu}{\mu_{i}-\mu_{i-1}} \Phi\left(x, \mu_{i-1}\right)
$$

An efficient quadrature must obey several criteria. For example, it must be invariant by projection: for the $1 D$ case, it is expressed by a reflective symmetry such that if the direction $\mu_{i}$ is kept, $-\mu_{i}$ should also be so as not to bias the current in

[^186]a given direction rather than the opposite. Besides, the first flux moment is the scalar flux which is positive for any spatial and angular domains:
$$
\Phi(x)=2 \pi \sum_{i=1}^{N} \varpi_{i} \Phi\left(x, \mu_{i}\right)
$$

This positive flux condition can be ensured by imposing positive weights, which is not necessarily the case in all quadratures. The Gauss quadrature made up with the roots of the Legendre polynomial is particularly well-suited for this purpose. Figure 9.3 illustrates a Gauss quadrature applied to the $S_{6}$ discretization. The quadratures for odd $n$ contain the direction $\pi / 2$ which has a zero cosine, and may lead to numerical problems in the numerical solution of the angularly discretized equation. This is why only even order quadratures are used. The weights are normalized such that:

$$
\sum_{i=1}^{n} \varpi_{i}=\int_{-1}^{+1} d \mu=2
$$

The expansion order can be very high and close to a spatial discontinuity, or a flux discontinuity for the direction $\mu=0$. In this case, space can be separated as two mirror sub-spaces for $\mu>0$ and $\mu<0$, for which a separate Gauss quadrature is applied. This technique is also applied in the $P_{n}$ method and is called the double $P_{n}$ or Yvon's method from the name of its inventor, and will be discussed later on. In $3 D$ geometry, two angles are required to define a direction. Let $\mu, \eta, \varepsilon$ be the


Fig. 9.3 Gauss quadrature for the $S_{6}$ discretization in $1 D$ geometry


Fig. 9.4 Symmetric quadrature for $S_{8}$ from (Lewis and Miller 1993)
cosines of the angles between the direction and the unit vectors of the $0 x y z$ basis. For a unit sphere (Fig. 9.4), these cosines are related as:

$$
\begin{equation*}
\text { Normalization condition: } \quad \mu^{2}+\eta^{2}+\varepsilon^{2}=1 \tag{9.2}
\end{equation*}
$$

For a symmetric quadrature, the retained values must be invariant by a $\pi / 2$ rotation and by symmetry wrt any plane of the reference frame. It can be shown (Duderstadt and Martin 1979), by considering an octant of the sphere with positive cosine, and expressing the normalization condition (Eq. 9.2) for the cosines of all directions with the same $\mu_{i}$, that these $\mu_{i}$ depend only on the first value $\mu_{1}$ and the index $i$ of the mesh as:

$$
\mu_{i}=\mu_{1}+\frac{2\left(1-3 \mu_{1}^{2}\right)}{n-2}(i-1)
$$

This is due to the fact that by numbering these values conveniently, the following relations are found by symmetry: $\left(\mu_{i}\right)_{i=1, n}=\left(\eta_{i}\right)_{i=1, n}=\left(\varepsilon_{i}\right)_{i=1, n}$. Thus, the directions can be concentrated towards the poles $(\mu= \pm 1)$ by choosing a small $\mu_{1}$
or close to the equator $(\mu=0)$ with a large $\mu_{1}$ (but less than $1 / \sqrt{3}$ according to the formula for the computation of the $\mu_{i}$ ). As for the $l D$ geometry, the weights are normalized on a quarter of the sphere $(-1 \leq \mu+1)$ as:

$$
\sum_{i=1}^{n(n+1)} \varpi_{i}=2
$$

The boundary conditions can be zero incoming flux at the surface of the medium [Mark conditions from C.F. Mark (Stamm'ler and Abbate 1983, p. 157)]:

$$
\Phi\left(\vec{r}_{S}, \vec{\Omega}_{i}\right)=0 \quad \text { for } \quad \vec{\Omega}_{i} \cdot \vec{n}>0
$$

Examples of dedicated S8 and S10 quadratures are shown in Figs. 9.5 and 9.6.

### 9.2 Exact $S_{n}$ Method

In 1979, Takahashi et al. ${ }^{7}$ introduced the exact $S_{n}$ method also called the $I^{*}$ method, which is a more precise formulation of the $S_{n}$ method. Let the equations in plane geometry without source be:

$$
\mu_{k} \frac{\partial \Phi_{k}}{\partial x}+\Sigma_{t, g} \Phi_{g}\left(x, \mu_{k}\right)=\sum_{h=1}^{G} \sum_{l=1}^{K} \omega_{l} \Sigma_{s}(h \rightarrow g, l \rightarrow k) \Phi_{h}\left(\mu_{l}\right)
$$

where $l$ is the index of the discretization of the quadrature and $h$ the index for the energy groups. The $S_{n}$ exact approach consists in expanding the differential scattering cross section with $I^{*}$ integrals defined as:

$$
\Sigma_{s}(h \rightarrow g, l \rightarrow k)=\sum_{m=1}^{M} \Sigma_{s}(h \rightarrow g, m) I^{*}(k, l, m)
$$

such that: $I^{*}(k, l, m)=\frac{1}{W_{k} W_{l} W_{m}} \iiint I^{*}\left(\mu, \mu^{\prime}, \gamma\right) d \mu d \mu^{\prime} d \gamma$,

$$
\begin{gathered}
W_{k}=\mu_{k+1 / 2}-\mu_{k-1 / 2}, W_{l}=\mu_{l+1 / 2}-\mu_{l-1 / 2}, W_{m}=\gamma_{m+1 / 2}-\gamma_{m-1 / 2} \\
I^{*}\left(\mu, \mu^{\prime}, \gamma\right)=\left\{\begin{array}{l}
\frac{1}{\pi \sqrt{D\left(\mu, \mu^{\prime}, \gamma\right)}} \\
0 \text { for } D<0
\end{array} \text { with } D\left(\mu, \mu^{\prime}, \gamma\right)=1-\mu^{2}-\mu^{\prime 2}-\gamma^{2}+2 \mu \mu^{\prime} \gamma\right.
\end{gathered}
$$

[^187]

Schematic view of the 24 backward directions of the S 8 full symmetric quadrature Description des 24 directions vers l'arrière de la quadrature 58 totalement symétrique


Schematic view of the 24 forward directions of the S8 full symmetric quadrature Description des 24 directions vers l'avant de la quadrature $\mathbf{S 8}$ totalement symétrique

Fig. 9.5 Fully symmetric S8 quadrature


Schematic view of the 35 backward directions of the S10 forward peaked biased quadrature Représentation des 35 directions vers l'arrière de la quadrature S10 biaisée vers l'avant


Schematic view of the 65 forward directions of the S10 forward peaked biased quadrature Représentation des 65 directions biaisées vers l'avant de la quadrature S10

Fig. 9.6 S10 quadrature biased forward. It better takes into account anisotropic scattering in light nuclei such as water (used by SCK MOL for the "concrete" benchmark in the BR1 reactor)
$\gamma$ is the cosine of the scattering angle in the laboratory frame. These integrals satisfy:

$$
\int_{-1}^{+1} I^{*}\left(\mu, \mu^{\prime}, \gamma\right) d \mu=\int_{-1}^{+1} I^{*}\left(\mu, \mu^{\prime}, \gamma\right) d \mu^{\prime}=\int_{-1}^{+1} I^{*}\left(\mu, \mu^{\prime}, \gamma\right) d \gamma=1
$$

The advantage of this method is that the integrals $I^{*}(k, l, m)$ can be computed analytically. ${ }^{8}$ This method is faster than the standard $S_{n}$ method.

### 9.3 Legendre Polynomial Method

### 9.3.1 Theory and Application to 1D Transport

(Clark and Hansen 1964, p. 184; Soodak et al. 1962, p. 106; Stacey 2001, p. 331; Stamm'ler and Abbate 1983, p. 18).
L. Gratton (1937) first attempted to represent the particle distribution in a multiple scattering problem with Legendre polynomials ${ }^{9}$ or the moments method as it was called back in the 1950's (Goldstein 1959, p. 265; Shimizu and Aoki 1972, p. 8). It was then employed by S. Chandrasekhar to the radiative transfer problem (1944). In 1951, M. C. Wang and E. Guth demonstrated (with notations very similar to those in neutronics) the equivalence of the exact solution of the integrodifferential form of the Boltzmann equation with anisotropic scattering by the flux approximation by expansion on the Legendre polynomial basis truncated at order $n$ and the Gauss quadrature of order $n+1$ (Electron physics 1954, p. 39).

The scattering law anisotropy can be modeled by expanding the differential scattering cross section on the Legendre polynomial basis $P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)$ where $\vec{\Omega} \cdot \vec{\Omega}^{\prime}$ is the scattering angle cosine:

$$
\Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{1}{4 \pi} \sum_{l=0}^{\infty}(2 l+1) \Sigma_{s, l}(\vec{r}) P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)
$$

where the coefficients of the expansion (called $l$ order moments) are given by:

[^188]$$
\Sigma_{s, l}(\vec{r})=\int_{4 \pi} d \vec{\Omega} \int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \cdot d \vec{\Omega}^{\prime}=2 \pi \int_{-1}^{+1} \Sigma_{s}\left(\vec{r}, \mu_{0}\right) P_{l}\left(\mu_{0}\right) d\left(\mu_{0}\right)
$$

It is not surprising that the cross section moments, which are mathematical coefficients, can be eventually negative. This is the case for instance of fifth order moments for the iron cross section for energies about 1 MeV , as indicated by (Foderaro 1971, p. 387). The possible expansion of the slowing-down operator with the scalar product $\mu_{0}=\vec{\Omega} \cdot \vec{\Omega}^{\prime}$ induces the fact this operator is invariant by rotation. It is recalled that the Legendre polynomials are defined by a recurrence relation (Hochstadt 1973, p. 7):

Recurrence formula for Legendre polynomials:

$$
\begin{equation*}
\mu P_{l}(\mu) \frac{l+1}{2 l+1} P_{l+1}(\mu)+\frac{l}{2 l+1} P_{l-1}(\mu) \quad \text { for } l \geq 1 \tag{9.3}
\end{equation*}
$$

The derivative of a Legendre polynomial can be easily computed as:

$$
\left(1-\mu^{2}\right) \frac{d P_{l}(\mu)}{d \mu}=(l+1)\left[\mu P_{l}(\mu)-P_{l+1}(\mu)\right]
$$

The first Legendre polynomials are:

$$
\begin{cases}P_{0}(\mu)=1 & P_{3}(\mu)=\frac{1}{2}\left(5 \mu^{3}-3 \mu\right) \\ P_{1}(\mu)=\mu & P_{4}(\mu)=\frac{1}{8}\left(35 \mu^{4}-30 \mu^{2}+3\right) \\ P_{2}(\mu)=\frac{1}{2}\left(3 \mu^{2}-1\right) & P_{5}(\mu)=\frac{1}{8}\left(65 \mu^{5}-70 \mu^{3}+15 \mu\right)\end{cases}
$$

However, their main property is that they are orthogonal, i.e.:

$$
\int_{-1}^{+1} P_{l}(\mu) P_{m}(\mu) d \mu=\frac{2}{2 l+1} \delta_{l m}
$$

or by integrating angularly as:
Orthogonality of the Legendre polynomials:

$$
\begin{equation*}
\int_{4 \pi} P_{l}(\mu) P_{m}(\mu) d \vec{\Omega}=2 \pi \int_{0}^{\pi} P_{l}(\mu) P_{m}(\mu) \sin \theta d \theta=\frac{4 \pi}{2 l+1} \delta_{l m} \tag{9.4}
\end{equation*}
$$

Thus, the Legendre polynomials form a complete basis for functions defined on the range $[-1,+1]$. For the first order expansion $(l=0)$ and since $P_{0}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=1$, the differential scattering cross section moment is obtained:

Zeroth moment of the differential scattering cross section (isotropic):

$$
\begin{align*}
\Sigma_{s, 0}(\vec{r}) & =\int_{4 \pi} d \vec{\Omega} \int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) P_{0}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} \\
& =\int_{4 \pi} d \vec{\Omega} \int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} \equiv \Sigma_{s}(\vec{r}) \tag{9.5}
\end{align*}
$$

The mean cosine of the scattering angle is defined as:
Mean cosine of the scattering angle:

$$
\begin{equation*}
\frac{\overline{\mu_{0}}(\vec{r})=\int \Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \vec{\Omega} \cdot \vec{\Omega}^{\prime} d\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)}{\Sigma_{s}(\vec{r})} \tag{9.6}
\end{equation*}
$$

In several works, the mean cosine of the scattering angle is coined as $\bar{\mu}$, we have preferentially employed $\overline{\mu_{0}}$ as in (Blaquière 1962), to avoid any confusion with $\mu=\vec{\Omega} \vec{x}=\cos \theta$. Since $P_{1}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\vec{\Omega} \cdot \vec{\Omega}^{\prime}=\mu_{0}$, for the first moment of the scattering cross section, the following equation is reached:

First moment of the differential scattering cross section:

$$
\begin{equation*}
\Sigma_{s, 1}(\vec{r})=\int \Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) P_{1}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) d\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\overline{\mu_{0}}(\vec{r}) \Sigma_{s}(\vec{r}) \tag{9.7}
\end{equation*}
$$

To allow for the energy variable, the differential cross section wrt angle and energy is expressed as:

$$
\Sigma_{s}\left(\vec{r}, E^{\prime} \rightarrow E, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{1}{4 \pi} \sum_{l=0}^{\infty}(2 l+1) \Sigma_{s, l}\left(\vec{r}, E^{\prime} \rightarrow E\right) P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)
$$

If collisions are assumed isotropic, the latter is simplified as:

$$
\Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{1}{4 \pi} \Sigma_{s, 0}(\vec{r})
$$

Thus, the differential scattering cross section no longer depends on the scattering angle and its integration over the unit sphere ( $4 \pi$ steradians) results in the isotropic scattering cross section. If the collision law is assumed to be linearly anisotropic with $\mu$, only the first moment of the differential cross section is retained, i.e.:

Linearly varying collision law: $\quad \Sigma_{s}\left(\vec{r}, \vec{\Omega} . \vec{\Omega}^{\prime}\right)=\frac{1}{4 \pi}\left[\Sigma_{s, 0}(\vec{r})+3 \mu \Sigma_{s, 1}(\vec{r})\right]$

$$
\begin{equation*}
=\frac{1+3 \mu \overline{\mu_{0}}}{4 \pi} \Sigma_{s, 0}(\vec{r}) \tag{9.8}
\end{equation*}
$$

On the other hand, the fission source term is always assumed isotropic. In practice, the expansion of the differential cross section is finite and truncated at order $n$ :

$$
\Sigma_{s}\left(\vec{r}, \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{1}{4 \pi} \sum_{l=0}^{n}(2 l+1) \Sigma_{s, l}(\vec{r}) P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)
$$

The Legendre polynomials with the scattering angle $P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)$ are more practical for our use if expressed in terms of the directions $\vec{\Omega}$ and $\vec{\Omega}^{\prime}$. Using the additivity formula, the Legendre polynomials can be decomposed into (complex) spherical harmonics $Y_{n}^{m}(\vec{\Omega})$ and their conjugate $\overline{Y_{n}^{m}(\vec{\Omega})}$ :

Additive property of the spherical harmonics:

$$
\begin{equation*}
P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{4 \pi}{2 l+1} \sum_{m=-1}^{m=+1} \overline{Y_{l}^{m}(\vec{\Omega})} Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right)=\frac{4 \pi}{2 l+1} \sum_{m=-1}^{m=+1} Y_{l}^{m}(\vec{\Omega}) \overline{Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right)} \tag{9.9}
\end{equation*}
$$

It can be noted that the second part of the equation which is the conjugate of the first part is justified since the corresponding Legendre polynomial is a real number, and the conjugate of a real number is itself. The scattering source is thus written as:

$$
\begin{align*}
& \int_{4 \pi} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} \\
& \quad=\int_{4 \pi} \frac{1}{4 \pi} \sum_{l=0}^{n}(2 l+1) \Sigma_{s, l}(\vec{r})\left(\frac{4 \pi}{2 l+1} \sum_{m=-1}^{m=+1} Y_{l}^{m}(\vec{\Omega}) \overline{Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right)}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} \tag{9.10}
\end{align*}
$$

With the hypothesis that the flux can also be expanded into spherical harmonics:

$$
\Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)=\sum_{l=0}^{l=+\infty} \sum_{m=-1}^{m=+1} \Phi_{l}^{m}(\vec{r}) Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right)
$$

the orthogonality property of these functions can be applied as follows:

$$
\int_{4 \pi} Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right) \overline{Y_{l^{\prime}}^{m \prime}\left(\overrightarrow{\Omega^{\prime}}\right)} d \overrightarrow{\Omega^{\prime}}=\delta_{l l^{\prime}} \delta_{m m^{\prime}}
$$

The flux expansion is injected in Eq. (9.10), and the scattering source term contains the flux moments after orthogonal terms have been cancelled out:

$$
\int_{4 \pi} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}=\sum_{l=0}^{m} \Sigma_{s, l}(\vec{r}) \sum_{m=-1}^{m=+1} Y_{l}^{m}(\vec{\Omega}) \Phi_{l}^{m}(\vec{r})
$$

In $1 D$, the flux is logically expressed with Legendre polynomials which are the form of the spherical harmonics in $1 D$. It can be noted that in this expression, the cosine of the incident neutron angle $\mu=\cos \theta=\vec{\Omega} \vec{x}$ is used, and not that of the scattering angle:

$$
\Phi(x, \vec{\Omega})=\frac{1}{4 \pi} \sum_{l=0}^{\infty}(2 l+1) \Phi_{l}(x) P_{l}(\vec{\Omega} \cdot \vec{x})=\frac{1}{4 \pi} \sum_{l=0}^{\infty}(2 l+1) \Phi_{l}(x) \sqrt{\frac{4 \pi}{2 l+1}} Y_{l}^{0}(\vec{\Omega})
$$

since the plane spherical harmonics $(m=0): Y_{l}^{0}(\vec{\Omega})=\sqrt{(2 l+1) /(4 \pi)} P_{l}(\vec{\Omega} \cdot \vec{x})$.
Although the plane spherical harmonics $Y_{l}^{0}(\vec{\Omega})$ is introduced somewhat artificially here, it will be justified further in the application of the model in $l D$ geometry for the angular integration in plane geometry. The flux is written in terms of $\mu$ and by multiplying by $2 \pi$ (by integration over the azimuthal angle $\varphi)^{10}$ :

[^189] moments, i.e.:
\[

\left\{$$
\begin{array}{c}
\Phi(x, \mu)=\sum_{l=0}^{\infty} \Phi_{l}(x) P_{l}(\mu) \\
\Phi_{l}(x)=\frac{2 l+1}{2} \int_{-1}^{+1} \Phi_{l}(x, \mu) P_{l}(\mu) d \mu
\end{array}
$$\right.
\]

These notations, although perfectly consistent, are nonetheless less convenient since the scalar flux $\Phi_{0}(x)$ is equal to half the integrated flux $\Phi(x)$ and that $\vec{\Phi}_{1}(x)$ is equal to $3 \vec{J}(x) / 2$, which are less easily recalled. Thus, just like (Blaquière 1962; Barjon 1993; Lewis and Miller 1993), we have chosen to extract the coefficient $2 l+1$ from the flux moments, as well as from the scattering cross section. Besides, it should also be noted that the famous numerical transport reference work (Lewis and Miller 1993) has chosen not to divide the angular flux by 2 and adds this factor to the coefficients of the moments as follows:

$$
\left\{\begin{array}{l}
\Phi(x, \mu)=\sum_{l=0}^{\infty}(2 l+1) \Phi_{l}(x) P_{l}(\mu) \\
\Phi_{l}(x)=\frac{1}{2} \int_{-1}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu
\end{array}\right.
$$

$P_{\infty}$ flux expansion: $\Phi(x, \mu)=2 \pi \Phi(x, \vec{\Omega})=\frac{1}{2} \sum_{l=0}^{\infty}(2 l+1) \Phi_{l}(x) P_{l}(\mu)$
with the flux moments:
Notations: $\forall l \quad \Phi_{l}(x)=\int_{-1}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu$ and $\Phi_{0}(x)=\int_{-1}^{+1} \Phi(x, \mu) d \mu$
With these notations, the flux moments are expressed with the different integration variables as:

Flux moment:

$$
\begin{align*}
\Phi_{l}(x) & =\int_{\theta=0}^{\theta=\pi} \Phi(x, \cos \theta) P_{l}(\cos \theta) \sin \theta d \theta=\int_{\theta=0}^{\theta=\pi} 2 \pi \Phi(x, \vec{\Omega}) P_{l}(\vec{\Omega} \cdot \vec{x}) \sin \theta d \theta \\
& =\int_{\theta=0}^{\theta=\pi} \Phi(x, \vec{\Omega}) P_{l}(\vec{\Omega} \cdot \vec{x}) \int_{\varphi=0}^{\varphi=2 \pi} \underbrace{\sin \theta d \theta d \varphi}_{d \vec{\Omega}}=\int_{4 \pi} \Phi(x, \vec{\Omega}) P_{l}(\vec{\Omega} \cdot \vec{x}) d \vec{\Omega} \tag{9.13}
\end{align*}
$$

For $P_{0}(\vec{\Omega}, \vec{x})=1$, the integral of the scalar flux, i.e. the integrated flux also called the scalar flux is obtained, and corresponds to the zeroth flux moment:

$$
\Phi_{0}(x)=\int_{4 \pi} \Phi(x, \vec{\Omega}) d \vec{\Omega} \equiv \Phi(x)
$$

The Eq. (9.10) simplifies to:

$$
\begin{aligned}
& \int_{\overrightarrow{\Omega^{\prime}} \in 4 \pi} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \cdot \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}= \\
& \int_{\vec{\Omega}^{\prime} \in 4 \pi} \frac{1}{4 \pi} \sum_{l=0}^{n}(2 l+1) \Sigma_{s, l}(\vec{r})\left[\frac{4 \pi}{2 l+1} \sum_{m=-l}^{m=+l} \overline{Y_{l}^{m}\left(\overrightarrow{\Omega^{\prime}}\right)} Y_{l}^{m}(\vec{\Omega})\right]\left[\frac{1}{4 \pi} \sum_{p=0}^{\infty}(2 p+1) \Phi_{p}(x) \sqrt{\frac{4 \pi}{2 p+1}} Y_{p}^{0}\left(\vec{\Omega}^{\prime}\right)\right] d \vec{\Omega}^{\prime}
\end{aligned}
$$

Using the orthogonality relations for the spherical harmonics, only the terms $m=0$ are conserved in the expansion of the Legendre polynomials with the additivity formula of the spherical harmonics. This equation is hence simplified as:

$$
\begin{aligned}
\int_{\vec{\Omega}^{\prime} \in 4 \pi} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \cdot \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} & =\sum_{l=0}^{n} \frac{(2 l+1)}{4 \pi} \Sigma_{s, l}(\vec{r}) \Phi_{l}(x) \underbrace{\sqrt{\frac{4 \pi}{2 l+1}} Y_{l}^{0}(\vec{\Omega})}_{p_{l}(\mu)} \\
& =\sum_{l=0}^{n} \frac{(2 l+1)}{4 \pi} \Sigma_{s, l}(\vec{r}) \Phi_{l}(x) P_{l}(\vec{\Omega} \cdot \vec{x})
\end{aligned}
$$

The different expressions lead to the classical time-independent $l D$ transport equation:
$1 D \operatorname{transport~equation:~} \mu \frac{\partial \Phi(x, \mu)}{\partial x}+\Sigma_{t}(x) \Phi(x, \mu)$

$$
\begin{equation*}
=\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} \Sigma_{s, l}(x) P_{l}(\mu) \Phi_{l}(x)+S(x, \mu) \tag{9.14}
\end{equation*}
$$

The source $S(x, \mu)$ is written as the integral of the multiplication rate over energy and angle for a multiplying medium without independent sources. With the cosine of the angle between vectors $\vec{\Omega}$ and $\vec{\Omega}^{\prime}$ as $\mu_{0} \equiv \cos \psi$, we obtain:

$$
S(x, \mu)=\frac{1}{2 \pi} \int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \int_{\varphi_{2}=0}^{\varphi_{2}=2 \pi} d \varphi_{2} \nu \Sigma_{f}\left(x, \mu_{0}\right) \Phi\left(x, \mu^{\prime}\right)
$$

The neutron production cross section can also be expanded with Legendre polynomials:

$$
\nu \Sigma_{f}\left(x, \mu_{0}\right)=\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} \nu \Sigma_{f, l}(x) P_{l}\left(\mu_{0}\right)
$$

and, it is usually assumed that this cross section is isotropic, thereby keeping only the first term of the expansion. Therefore:

$$
\begin{gather*}
\nu \Sigma_{f}\left(x, \mu_{0}\right)=\frac{1}{2} \nu \Sigma_{f, 0}(x) \text { with } \\
\nu \Sigma_{f}(x)=\int_{\mu_{0}=-1}^{\mu_{0}=+1} \nu \Sigma_{f}\left(x, \mu_{0}\right) d \mu_{0}=\int_{\mu_{0}=-1}^{\mu_{0}=+1} \frac{1}{2} \nu \Sigma_{f, 0}(x) d \mu_{0}=\nu \Sigma_{f, 0} \tag{x}
\end{gather*}
$$

It can be deduced that:

$$
\begin{aligned}
S(x, \mu) & =\frac{1}{2 \pi} \int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \int_{\varphi_{2}=0}^{\varphi_{2}=2 \pi} d \varphi_{2} \nu \Sigma_{f}\left(x, \mu_{0}\right) \Phi\left(x, \mu^{\prime}\right) \\
& =\frac{1}{2} \nu \Sigma_{f, 0}(x) \frac{1}{2 \pi} \int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \int_{\varphi_{2}=0}^{\varphi_{2}=2 \pi} d \varphi_{2} \Phi\left(x, \mu^{\prime}\right) \\
& =\frac{1}{2} \nu \Sigma_{f, 0}(x) \underbrace{\int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \Phi\left(x, \mu^{\prime}\right)}_{\Phi(x)}
\end{aligned}
$$

i.e.:

$$
S(x, \mu)=\frac{1}{2} \nu \Sigma_{f, 0} \quad(x) \Phi(x)
$$

This angular source satisfies:

$$
\int_{\mu=-1}^{\mu=+1} d \mu S(x, \mu)=\int_{\mu=-1}^{\mu=+1} d \mu \frac{1}{2} \nu \Sigma_{f, 0}(x) \Phi(x)=\nu \Sigma_{f, 0}(x) \Phi(x)
$$

It should be noted that some authors write the transport equation using the flux per unit solid angle (steradian) defined by:

$$
\phi(x)_{\left[n / \mathrm{cm}^{2} / s / \text { steradian }\right]}=\frac{1}{4 \pi} \int_{\mu=-1}^{\mu=+l} d \mu \int_{\varphi=0}^{\varphi=2 \pi} d \varphi \phi(x, \mu, \varphi)=\frac{1}{2} \int_{\mu=-1}^{\mu=+1} d \mu \phi(x, \mu)
$$

This result holds by assuming a revolution symmetry about the $0 x$ axis for the medium. Thus, the flux $\phi(x, \mu, \varphi)$ is independent of $\varphi$ and a $1 / 2$ factor is introduced. Equation (9.14) for $\phi(x, \mu)$ is expressed by omitting the $1 / 2$ factor:

$$
\begin{aligned}
s(x, \mu) & =\frac{1}{2 \pi} \int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \int_{\varphi_{2}=0}^{\varphi_{2}=2} d \varphi_{2} \nu \Sigma_{f}\left(x, \mu_{0}\right) \phi\left(x, \mu^{\prime}\right) \\
& =\nu \Sigma_{f, 0}(x) \underbrace{\frac{1}{2} \int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \phi\left(x, \mu^{\prime}\right)}_{\phi(x)}=\nu \Sigma_{f, 0}(x) \phi(x)
\end{aligned}
$$

Even though the latter seems inconsistent with the result for $\Phi(x, \mu)$, it should be recalled that the integration of the following equation $w r t \mu$ :

$$
\mu \frac{\partial \phi(x, \mu)}{\partial x}+\Sigma_{t}(x) \phi(x, \mu)=\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} \Sigma_{s, l}(x) P_{l}(\mu) \phi_{l}(x)+s(x, \mu)
$$

includes the term $\int_{\mu=-1}^{\mu=+1} d \mu \phi(x, \mu)=2 \phi(x)$ which compensates the lack of the $1 / 2$ factor. Both notations are hence consistent.

The scattering term $\int_{4 \pi} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}$ can also be simplified without using the expansion on the spherical harmonics. Instead, the additivity formula is applied directly for the Legendre polynomials thereby introducing the associated Legendre functions (Fig. 9.7).

If applied to a $l D$ geometry, the differential scattering cross section is expressed using the additivity formula for the spherical harmonics. Using the sum formula for angles, the cosine of the scattering angle $\mu_{0}=\vec{\Omega} \cdot \vec{\Omega}^{\prime}=\cos \psi$, that of the incident direction $\mu=\vec{\Omega} \cdot \vec{x}=\cos \theta_{1}$ and that of the outgoing direction $\mu^{\prime}=\vec{\Omega}^{\prime} \cdot \vec{x}=\cos \theta_{2}$ are related as follows:

Additivity formula for the Legendre polynomials:

$$
\begin{gather*}
\mu_{0} \equiv \cos \psi=\cos \theta_{1} \cos \theta_{2}+\sin \theta_{1} \sin \theta_{2}+\cos \left(\varphi_{1}-\varphi_{2}\right) \\
P_{l}\left(\mu_{0}\right)=P_{l}(\mu) P_{l}\left(\mu^{\prime}\right)+2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)} P_{l}^{m}(\mu) P_{l}^{m}\left(\mu^{\prime}\right) \cos \left(m\left(\varphi_{1}-\varphi_{2}\right)\right) \tag{9.15}
\end{gather*}
$$

In this equation, $P_{l}^{m}(\mu)$ is the associated Legendre function (Robin 1959), defined such that:

Fig. 9.7 Angles used for the collision description


$$
P_{l}^{m}(\mu)=(-1)^{m}\left(1-\mu^{2}\right)^{\frac{m}{2}} \frac{d^{m} P_{l}(\mu)}{d \mu^{m}}
$$

The first few terms are written as: $P_{0}^{0}(\mu)=1, P_{1}^{0}(\mu)=\mu, P_{1}^{1}(\mu)=-\sqrt{\left(1-\mu^{2}\right)}$, $P_{2}^{0}(\mu)=\frac{1}{2}\left(3 \mu^{2}-1\right), P_{2}^{1}(\mu)=-3 \mu \sqrt{\left(1-\mu^{2}\right)}, P_{2}^{2}(\mu)=3\left(1-\mu^{2}\right)$.

With these results, the integration of the scattering rate is computed by substituting the flux and the cross section by their respective expansion:

$$
\begin{aligned}
& \int_{4 \pi} \Sigma_{S}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}=\int_{4 \pi} \sum_{l} \frac{2 l+1}{4 \pi} \Sigma_{s l}(x) P_{l}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime} \\
& =\int_{\varphi_{2}=0}^{\varphi_{2}=2 \pi} d \varphi_{2} \int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \sum_{l=1}^{n} \frac{2 l+1}{4 \pi} \Sigma_{s l}(x) P_{l}(\mu) P_{l}\left(\mu^{\prime}\right) \Phi\left(\vec{r}, \mu^{\prime}\right) \\
& \quad+\int_{\mu^{\prime}=-1}^{\mu^{\prime}=+1} d \mu^{\prime} \sum_{l} \frac{2 l+1}{4 \pi} \Sigma_{s l}(x)[2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)} P_{l}^{m}(\mu) P_{l}^{m}\left(\mu^{\prime}\right) \Phi\left(\vec{r}, \mu^{\prime}\right) \underbrace{\varphi_{\varphi_{2}=0}^{\varphi_{2}=2 \pi} d \varphi_{2} \cos \left(m\left(\varphi_{1}-\varphi_{2}\right)\right)}] \\
& =\sum_{l} \frac{2 l+1}{2} \Sigma_{s, l}(x) P_{l}(\mu) \Phi_{l}(x)
\end{aligned}
$$

By integration wrt $\varphi_{2}$, the terms with the associated Legendre functions cancel out. The remaining terms are the $t^{\text {th }}$ flux moments: $\Phi_{l}(x)=\int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) P_{l}\left(\mu^{\prime}\right) d \mu^{\prime}$. Thus, the same scattering term as Eq. (9.14) is obtained. The $P_{n}$ approximation consists in truncating the flux expansion at a finite order $n$ :

$$
\begin{equation*}
P_{n} \text { approximation of the flux: } \quad \Phi(x, \mu)=\frac{1}{2} \sum_{l=0}^{l=n}(2 l+1) \Phi_{l}(x) P_{l}(\mu) \tag{9.16}
\end{equation*}
$$

The even $l$ terms are usually called the $l^{\text {th }}$ order flux while the odd $l$ terms are called currents. The $\Phi_{1}$ term plays a pivotal role as it will be later seen that it corresponds to the current $J$ used in diffusion theory. This is also why the flux is sometimes written as:

$$
\Phi(x, \mu)=\frac{1}{2} \sum_{h=0}^{\frac{n-1}{2}}(4 h+1) \Phi_{2 h}(x) P_{2 h}(\mu)+(4 h+3) \vec{\psi}_{2 h+1}(x) \cdot \vec{x} P_{2 h+1}(\mu)
$$

which separates the even and odd components clearly. An analysis of Eq. (9.14) shows that it is not necessary to expand the differential scattering cross section at orders higher than $n$ since $\Phi_{l>n}=0$. Thus, in practice, the differential scattering cross section is expanded at order $n$. An anisotropic source may also be expanded with Legendre polynomials. The polynomial expansion being a converging process,
the flux moments decay quickly and only the first terms can be retained. If restricted to the first term, the flux is given by:
$P_{1}$ flux approximation:

$$
\begin{equation*}
\Phi(x, \mu) \approx \frac{1}{2}\left[\Phi_{0}(x) P_{0}(\mu)+3 \Phi_{1}(x) P_{1}(\mu)\right]=\frac{1}{2}\left[\Phi_{0}(x)+3 \mu \Phi_{1}(x)\right] \tag{9.17}
\end{equation*}
$$

From the definition of $\Phi_{1}(x)=\int_{-1}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu=\int_{-1}^{+1} v n(x, \mu)$ $\cos \theta d(\cos \theta)$, it can be noted that this expression is simply the net number of neutrons that travel through a cross section of $1 \mathrm{~cm}^{2}$ surface area perpendicular to the $x$ axis. Therefore, this corresponds to the neutron current $J(x)$. The flux can hence be written in terms of current as:

$$
\Phi(x, \vec{\Omega})=\frac{1}{4 \pi}\left[\Phi_{0}(x)+3 \vec{\Omega} \cdot \vec{J}(x)\right] \quad \text { or even: } \quad \Phi(x, \mu)=\frac{1}{2}\left[\Phi_{0}(x)+3 \mu J(x)\right]
$$

Injecting Eq. (9.17) into Eq. (9.14), we obtain (after simplifying by 1/2):

$$
\begin{aligned}
& \mu \frac{\partial \Phi_{0}(x)}{\partial x}+3 \mu^{2} \frac{\partial J(x)}{\partial x}+\Sigma_{t} \Phi_{0}(x)+3 \mu \Sigma_{t} J(x) \\
& =\Sigma_{s, 0} \int_{-1}^{+1}\left[\Phi_{0}(x)+3 \mu^{\prime} J(x)\right] d \mu^{\prime} \\
& \quad+3 \Sigma_{s, 1} \int_{-1}^{+1} \mu^{\prime}\left[\Phi_{0}(x)+3 \mu^{\prime} J(x)\right] d \mu^{\prime}+2 S(x, \mu)
\end{aligned}
$$

It can be pointed out that the orders higher than 1 for the scattering cross section cancel out due to the truncated flux. The integral calculation leads to the relation between the direct flux and the neutron current:

$$
\text { Flux-current equation: } \begin{array}{r}
\mu \frac{\partial \Phi_{0}(x)}{\partial x}+3 \mu^{2} \frac{\partial J(x)}{\partial x}+\Sigma_{t} \Phi_{0}(x)+3 \mu \Sigma_{t} J(x) \\
=\Sigma_{s, 0} \Phi_{0}(x)+3 \mu \Sigma_{s, 1} J(x)+2 S(x, \mu) \tag{9.18}
\end{array}
$$

Integrating Eq. (9.18) wrt $\mu$ over $[-1,+1]$, the following conservation equation is reached:

$$
\frac{\partial J(x)}{\partial x}+\Sigma_{t} \Phi_{0}(x)=\Sigma_{s, 0} \Phi_{0}(x)+\int_{-1}^{+1} S(x, \mu) d \mu
$$

where $\int_{-1}^{+1} S(x, \mu) d \mu=S(x)$ is the total source intensity. This balance equation describes the neutron balance in a volume element. It can be extended in $3 D$ as:

Neutron conservation equation: $\operatorname{div} \vec{J}(\vec{r})+\Sigma_{t}(\vec{r}) \Phi_{0}(\vec{r})=\Sigma_{s, 0} \Phi_{0}(\vec{r})+S(\vec{r})$
Multiplying Eq. (9.18) by $P_{1}(\mu)=\mu$ and integrating over $[-1,+1]$ leads to:

$$
\frac{\partial \Phi_{0}(x)}{\partial x}+3 \Sigma_{t} J(x)=3 \Sigma_{s, 1} J(x)
$$

or:

$$
J(x)=-\frac{1}{3\left(\Sigma_{t}-\Sigma_{s, 1}\right)} \frac{\partial \Phi_{0}(x)}{\partial x}
$$

Since:

$$
\Sigma_{s, 1}=\int_{-1}^{+1} P_{1}\left(\mu_{0}\right) \Sigma_{s}\left(\mu_{0}\right) d \mu_{0}=\int_{-1}^{+1} \mu_{0} \Sigma_{s}\left(\mu_{0}\right) d \mu_{0} \equiv \overline{\mu_{0}} \Sigma_{s, 0}
$$

It results in the formula that relates the current to the flux gradient similar to the Fick's law applied to chemical diffusion or the Fourier law in heat conduction theory:

$$
\begin{equation*}
\text { Fick's law: } \quad J(x)=-\frac{1}{3\left(\Sigma_{t}-\overline{\mu_{0}} \Sigma_{s, 0}\right)} \frac{\partial \Phi_{0}(x)}{\partial x}=-D \frac{\partial \Phi_{0}(x)}{\partial x} \tag{9.20}
\end{equation*}
$$

Therefore, the $P_{1}$ expansion of the Boltzmann equation leads to Fick's law for the current and the flux with the proportionality coefficient, called the diffusion coefficient, being given as (Meghreblian and Holmes 1960, p. 342):

$$
\begin{equation*}
\text { Diffusion coefficient in } P_{1} \text { approximation: } \quad D \equiv \frac{1}{3\left(\Sigma_{t}-\overline{\mu_{0}} \Sigma_{s, 0}\right)} \tag{9.21}
\end{equation*}
$$

The $\Sigma_{t r} \equiv \Sigma_{t}-\overline{\mu_{0}} \Sigma_{s, 0}$ cross section is called the transport-corrected cross section or simply the transport cross section. The flux moments are computed by multiplying each term of Eq. (9.14) successively by $P_{l}(\mu), l=1$ to $n$ and by integrating on $[-1,+1]$ (after substituting the flux by its expansion). Integrating the first term leads to:

$$
\begin{aligned}
& \int_{-1}^{+1} P_{l}(\mu) \mu \frac{\partial \sum_{l^{\prime}=0}^{n} \frac{\left(2 l^{\prime}+1\right)}{2} \Phi_{l^{\prime}}(x) P_{l^{\prime}}(\mu)}{\partial x} d \mu \\
& \quad= \begin{cases}\frac{\partial \Phi_{1}(x)}{\partial x} & \text { for } l=0 \\
{\left[\frac{(l+1)}{2 l+1} \frac{\partial \Phi_{l+1}(x)}{\partial x}+\frac{l}{2 l+1} \frac{\partial \Phi_{l-1}(x)}{\partial x}\right]} & \text { for } 1 \leq l \leq n-1 \\
\frac{n}{2 n+1} \frac{\partial \Phi_{n-1}(x)}{\partial x} & \text { for } l=n\end{cases}
\end{aligned}
$$

using the recurrence relation for Legendre polynomials:

$$
\mu P_{l}(\mu)=\frac{l+1}{2 l+1} P_{l+1}(\mu)+\frac{l}{2 l+1} P_{l-1}(\mu) \quad \text { for } l \geq 1
$$

The integration of the second term is expressed as:

$$
\int_{-1}^{+1} P_{l}(\mu) \Sigma_{t}(x) \sum_{l^{\prime}=0}^{n} \frac{\left(2 l^{\prime}+1\right)}{2} \Phi_{l^{\prime}}(x) P_{l^{\prime}}(\mu) d \mu=\Sigma_{t}(x) \Phi_{l}(x)
$$

and the terms on the RHS are written as:

$$
\begin{aligned}
& \int_{-1}^{+1} d \mu P_{l}(\mu)[\sum_{l^{\prime}=0}^{l^{\prime}=n} \frac{2 l^{\prime}+1}{2} \Sigma_{s, l^{\prime}}(x) P_{l^{\prime}}(\mu) \underbrace{\int_{-1}^{+1} P_{l^{\prime}}\left(\mu^{\prime}\right) \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}}_{\Phi_{l}(x)}+S(x, \mu)] \\
& \quad=\Sigma_{s, l}(x) \Phi_{l}(x)+\int_{-1}^{+1} P_{l}(\mu) S(x, \mu) d \mu
\end{aligned}
$$

Hence, Eq. (9.14) can be written as:
$P_{\mathrm{n}}$ equation system discretized with flux moments:

$$
\left\{\begin{array}{l}
\frac{\partial \Phi_{1}(x)}{\partial x}+\Sigma_{t}(x) \Phi_{0}(x)=\Sigma_{s, 0}(x) \Phi_{0}(x)+\int_{-1}^{+1} P_{0}(\mu) S(x, \mu) d \mu  \tag{9.22}\\
\vdots \\
\frac{(l+1)}{2 l+1} \frac{\partial \Phi_{l+1}(x)}{\partial x}+\frac{l}{2 l+1} \frac{\partial \Phi_{l-1}(x)}{\partial x}+\Sigma_{t}(x) \Phi_{l}(x)=\Sigma_{s, l}(x) \Phi_{l}(x)+\int_{-1}^{+1} P_{l}(\mu) S(x, \mu) d \mu \\
\vdots \\
\frac{n}{2 n-1} \frac{\partial \Phi_{n}(x)}{\partial x}+\frac{n-1}{2 n-1} \frac{\partial \Phi_{n-2}(x)}{\partial x}+\Sigma_{t}(x) \Phi_{n-1}(x)=\Sigma_{s, n-1}(x) \Phi_{n-1}(x)+\int_{-1}^{+1} P_{n-1}(\mu) S(x, \mu) d \mu \\
\frac{n}{2 n+1} \frac{\partial \Phi_{n-1}(x)}{\partial x}+\Sigma_{t}(x) \Phi_{n}(x)=\Sigma_{s, n}(x) \Phi_{n}(x)+\int_{-1}^{+1} P_{n}(\mu) S(x, \mu) d \mu
\end{array}\right.
$$

The source expansion terms $S_{l}(x)=\int_{-1}^{+1} S(x, \mu) P_{l}(\mu) d \mu$ are given by:

$$
S(x, \mu)=\frac{1}{2} \sum_{l=0}^{l=n}(2 l+1) S_{l}(x) P_{l}(\mu)
$$

For an isotropic source, $S(x, \mu)=S(x,-\mu)=S_{0}(x) P_{0}(\mu) / 2=S_{0}(x) / 2$ which describes the fact that half the number of neutrons emitted by the source travel to the right of the slab source and the other half to the left.

The boundary conditions applied to the surface of the medium are called March$\mathrm{ak}^{11}$ boundary conditions for cases surrounded by vacuum (zero incoming current). The odd flux moments cancel out, especially the current, for incoming angles (Marchak 1959, p. 221):

$$
\int_{-1}^{0} P_{l}(\mu) \Phi\left(x_{S}, \mu\right) d \mu=0 \quad \text { for } \quad l=1,3,5, \ldots n
$$

This approach is identical to substituting the Legendre polynomials by $\mu^{l}$. If the case is symmetric (e.g. a slab with a symmetric source), symmetry considerations can be employed to describe the conditions explicitly on the flux moments at the slab center:

$$
\left\{\begin{array}{lll}
\Phi_{k}(0)=0 & k & \text { odd } \\
\left.\frac{\partial \Phi_{k}}{\partial x}\right|_{0}=0 & k & \text { even }
\end{array}\right.
$$

Injecting the $P_{n}$ flux expansion, the $P_{n}$ scattering cross section and the source in the angular transport equation (Eq. 9.14), the resulting equation is that where two polynomials in $\mu$ are obtained equal to each other:

$$
\begin{aligned}
\mu & \sum_{l=0}^{l=n} \frac{2 l+1}{2} \frac{\partial \Phi_{l}(x)}{\partial x} P_{l}(\mu)+\Sigma_{t}(x) \quad \sum_{l=0}^{l=n} \frac{2 l+1}{2} \Phi_{l}(x) P_{l}(\mu) \\
& =\sum_{l=0}^{l=n} \frac{2 l+1}{2} \Sigma_{s, l}(x) P_{l}(\mu) \Phi_{l}(x)+\sum_{l=0}^{l=n} \frac{2 l+1}{2} S_{l}(x) P_{l}(\mu)
\end{aligned}
$$

The even-flux equation is obtained by identification of the constant term (independent of $\mu$ ), which is supposed to be valid for the direction perpendicular to the $O \vec{x}$ axis $(\mu=0)$, i.e.:

[^190]$P_{n}$ transport equation at $\mu=0$ :
\[

$$
\begin{equation*}
\Sigma_{t}(x)\left[\sum_{k=0}^{k=n / 2} \frac{4 k+1}{2} \Phi_{2 k}(x) P_{2 k}(0)\right]=\sum_{k=0}^{k=n / 2} \frac{4 k+1}{2}\left(\Sigma_{s, 2 k}(x) \Phi_{2 k}(x)+S_{2 k}(x)\right) P_{2 k}(0) \tag{9.23}
\end{equation*}
$$

\]

We have implemented the fact that the constant part of the odd Legendre polynomials is equal to zero: $P_{2 k+1}(0)=0$. The above equation is physically inconsistent if the expansion is limited to a finite order, for instance by considering the $P_{1}$ expansion:

$$
\Sigma_{t}(x) \Phi_{0}(x)=\Sigma_{s, 0}(x) \Phi_{0}(x)+S_{0}(x)
$$

This equation is very surprising since it implies that the isotropic flux could be obtained by solving it with a local source, irrespective of the boundary conditions surrounding the position $x$. It should also be noted that a zero-source problem (e.g. by imposing a neutron current at an interface) leads to an inconsistent physical equation $\Sigma_{t}(x) \Phi_{0}(x)=\Sigma_{s, 0}(x) \quad \Phi_{0}(x)$ implying that $\Sigma_{t}(x)$ is equal to $\Sigma_{s, 0}(x)$, which is not the case except for a non-absorbing medium. Hence, the separation of the space and angle variables leads to nonsensical results if injected over in the initial angle-dependent equation owing to the limited-order expansion. Therefore, it should be noted that the method consists in cancelling the $n$ initial moments of the transport equation written as $H(\Phi(x, \mu))=0$. Yet, the gradient term $\mu \partial \Phi / \partial x$ leads to a polynomial form of the transport equation with degree $n+1$ assuming that the flux is truncated at order $n$, and can thus be expressed as:

$$
\begin{aligned}
& H(\Phi(x, \mu))=\sum_{l=0}^{l=n+1} \frac{2 l+1}{2} H_{l}(x) P_{l}(\mu)=0 \\
& H(\Phi(x, \mu))=0 \Rightarrow \sum_{l=0}^{l=n+1} \frac{2 l+1}{2} H_{l}(x) P_{l}(\mu)=0 \\
& \Leftrightarrow \begin{cases}\int_{-1}^{+1} P_{0}(\mu) \sum_{l=0}^{l=n+1} \frac{2 l+1}{2} H_{l}(x) P_{l}(\mu) d \mu=H_{0}(x) & \Rightarrow H_{0}(x)=0 \\
\int_{-1}^{+1} P_{1}(\mu) \sum_{l=0}^{l=n+1} \frac{2 l+1}{2} H_{l}(x) P_{l}(\mu) d \mu=H_{1}(x) & \Rightarrow H_{1}(x)=0 \\
\vdots \\
\int_{-1}^{+1} P_{n}(\mu) \sum_{l=0}^{l=n+1} \frac{2 l+1}{2} H_{l}(x) P_{l}(\mu) d \mu=H_{n}(x) & \Rightarrow H_{n}(x)=0 \\
\int_{-1}^{+1} P_{n+1}(\mu) \sum_{l=0}^{l=n+1} \frac{2 l+1}{2} H_{l}(x) P_{l}(\mu) d \mu=\frac{n+1}{2 n+3} \frac{\partial \Phi_{n}(x)}{\partial x} \neq 0\end{cases}
\end{aligned}
$$

To ensure that $H(\Phi(x, 0))=0$, the following condition must be satisfied:

$$
H_{n+1}(x)=\frac{n+1}{2 n+3} \frac{\partial \Phi_{n}(x)}{\partial x}=0
$$

An erroneous solution is thereby obtained where the last flux moment is constant for any situation. Thus, the $P_{n}$ solution reached by cancelling the $n$ first moments of the transport equation does not ensure that $H(\Phi(x, 0))=0$ (Eq. 9.23). Even if a source were present, coupled to the flux or not, the same conclusions hold. Increasing the order of the $P_{n}$ expansion means that Eq. (9.23) will have better chances of being satisfied, i.e. the method converges towards the exact solution. However, the "paradox" remains that no truncated expansion may truly satisfy the initial equation for each angular direction. Nevertheless, the $P_{n}$ method is very interesting as it leads to a tri-diagonal diffusion operator expressed in matrix form, and thus inhibits ray effects which are inherent to the $S_{n}$ method. It is costly in terms of computational times and led to the emergence of methods such as the $S P_{n}$ method. For $1 D$ geometries, studies have shown ${ }^{12}$ that the Legendre polynomials method was more efficient than the usual methods such as the collision probability method, the flux expansion in Taylor or Fourier series or the integration methods by Euler's method, trapezium rule or Gauss quadrature.

### 9.3.2 Multi-group 1D Transport and Diffusion Equivalence

The general multi-group equation (for $G$ groups) is written as:

$$
\begin{aligned}
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{g}(\vec{r}, \vec{\Omega})+\Sigma_{t, g} \Phi_{g}(\vec{r}, \vec{\Omega})=\sum_{g^{\prime}=1}^{g^{\prime}=G} \int_{\overrightarrow{\Omega^{\prime}}} \Sigma_{g^{\prime} \rightarrow g}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \Phi_{g^{\prime}}(\vec{r}, \vec{\Omega}) d \vec{\Omega}^{\prime} \\
+\chi_{g} \sum_{g^{\prime}=1}^{g^{\prime}=G} \int_{\vec{\Omega}^{\prime}} \nu \Sigma_{f, g^{\prime}}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) \Phi_{g^{\prime}}(\vec{r}, \vec{\Omega}) d \vec{\Omega}^{\prime}
\end{aligned}
$$

With the usual notations in this work, the projection of the $1 D$ problem on the $O x$ axis is:

[^191]\[

$$
\begin{aligned}
\mu \frac{\partial \Phi_{g}(x, \mu)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g}(x, \mu)= & \sum_{g^{\prime}=1}^{g^{\prime}=G} \frac{1}{2 \pi} \int_{\mu^{\prime}=1}^{\mu^{\prime}=+1} d \mu^{\prime} \int_{\varphi_{2}=0}^{\varphi_{2}=2 \pi} \Sigma_{g^{\prime} \rightarrow g}\left(x, \mu_{0}\right) \Phi_{g^{\prime}}\left(x, \mu^{\prime}\right) \\
& +\chi_{g} \sum_{g^{\prime}=1}^{g^{\prime}=G} \frac{1}{2} \Sigma_{f, g^{\prime}}(x) \Phi_{g^{\prime}}(x)
\end{aligned}
$$
\]

with $\Phi_{g}(x)=\int_{\mu=1}^{\mu=+1} \Phi_{g}(x, \mu) d \mu$
The scattering term is simplified by expanding the differential scattering cross section as:

$$
\Sigma_{g^{\prime} \rightarrow g}\left(x, \mu_{0}\right)=\frac{1}{2} \sum_{l=0}^{l=\infty}(2 l+1) \Sigma_{g^{\prime} \rightarrow g, l}(x) P_{l}\left(\mu_{0}\right)
$$

The addition formula for the Legendre polynomial (Eq. 9.15) is then applied to eliminate $\mu_{0}$ such that:

$$
\begin{aligned}
& \mu \frac{\partial \Phi_{g}(x, \mu)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g}(x, \mu) \\
& =\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} P_{l}(\mu) \sum_{g^{\prime}=1}^{g^{\prime}=G} \Sigma_{g^{\prime} \rightarrow g}(x) \int_{\mu^{\prime}=1}^{\mu^{\prime}=+1} d \mu^{\prime} P_{l}\left(\mu^{\prime}\right) \Phi_{g^{\prime}}\left(x, \mu^{\prime}\right)+\chi_{g} \sum_{g^{\prime}=1}^{g^{\prime}=G} \frac{1}{2} \Sigma_{f, g^{\prime}}(x) \Phi_{g^{\prime}}(x)
\end{aligned}
$$

The angular flux can also be expanded in Legendre polynomials as:

$$
\Phi_{g^{\prime}}\left(x, \mu^{\prime}\right)=\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} P_{l}\left(\mu^{\prime}\right) \Phi_{g^{\prime}, l}(x)
$$

Finally:
$1 D$ multi-group transport equation:

$$
\begin{align*}
\mu \frac{\partial \Phi_{g}(x, \mu)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g}(x, \mu)= & \sum_{l=0}^{l=\infty} \frac{2 l+1}{2} P_{l}(\mu) \sum_{g^{\prime}=1}^{g^{\prime}=G} \Sigma_{g^{\prime} \rightarrow g, l}(x) \Phi_{g^{\prime}, l}(x) \\
& +\chi_{g} \sum_{g^{\prime}=1}^{g^{\prime}=G} \frac{1}{2} \Sigma_{f, g^{\prime}}(x) \Phi_{g^{\prime}}(x) \tag{9.24}
\end{align*}
$$

The transfer cross section $\Sigma_{g^{\prime} \rightarrow g}$ depends on $\mu_{0}$ according to the studied case. This cross section describes all the collisions except fission, i.e. elastic scattering, inelastic scattering, $(n, 2 n),(n, 3 n)$ reactions, etc. Scattering reactions are assumed as being isotropic under a threshold energy estimated as $10 / A^{2 / 3} \mathrm{MeV}$, where $A$ is the nuclear mass of the target nuclide. For hydrogenated media, it is thus justified to assume that all elastic scatterings are isotropic even if there are scatterings with heavy nuclides such as uranium which are below 200 keV . On the other hand, inelastic scattering reactions are:

- Anisotropic for light nuclides such as hydrogen (but that reaction is fairly improbable in a $P W R$ since it is a threshold reaction at 10 MeV ),
- Isotropic with a slight error for structure nuclides such as iron or zirconium,
- Isotropic for heavy nuclides.

For one-group theory, the current can be related to the integrated flux gradient with the formula:

$$
J(x)=\Phi_{1}=-\frac{1}{3\left(\Sigma_{t}-\Sigma_{s, l}\right)} \frac{\partial \Phi_{0}(x)}{\partial x}
$$

By projecting the multi-group equation (Eq. 9.24) on the basis of Legendre polynomials and by integrating over $\mu$ from -1 to +1 , the flux moments are obtained as follows (without upscattering for anisotropic cross sections, with the assumption that $\left.\Sigma_{g}, \rightarrow g<g^{\prime}, l \geq 1=0\right)$ :

$$
\left\{\begin{array}{l}
\frac{\partial \Phi_{g, 1}(x)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g, 0}(x)=\sum_{g^{\prime}=1}^{g^{\prime}=G} \Sigma_{g^{\prime} \rightarrow g, 0}(x) \Phi_{g^{\prime}, 0}(x)+\chi_{g} \sum_{g^{\prime}=1}^{g^{\prime}=G} \Sigma_{f, g^{\prime}}(x) \Phi_{g^{\prime}}(x) \\
\frac{2}{3} \frac{\partial \Phi_{g, 2}(x)}{\partial x}+\frac{1}{3} \frac{\partial \Phi_{g, 0}(x)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g, 1}(x)=\sum_{\substack{g^{\prime}=1 \\
g^{\prime}=g}} \Sigma_{g^{\prime} \rightarrow g, 1}(x) \Phi_{g^{\prime}, 1}(x) \\
\frac{3}{5} \frac{\partial \Phi_{g, 3}(x)}{\partial x}+\frac{2}{5} \frac{\partial \Phi_{g, 1}(x)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g, 2}(x)=\sum_{g^{\prime}=g} \Sigma_{g^{\prime} \rightarrow g, 2}(x) \Phi_{g^{\prime}, 2}(x) \\
\frac{4}{7} \frac{\partial \Phi_{g, 4}(x)}{\partial x}+\frac{3}{7} \frac{\partial \Phi_{g, 2}(x)}{\partial x}+\Sigma_{t, g}(x) \Phi_{g, 3}(x)=\sum_{g^{\prime}=1}^{g^{\prime}=g} \Sigma_{g^{\prime} \rightarrow g, 2}(x) \Phi_{g^{\prime}, 3}(x) \\
\vdots \\
\vdots
\end{array}\right.
$$

The law that relates the current to the integrated flux gradient while neglecting the term $2 \partial \Phi_{g, 2}(x) / 3 \partial x$ leads to the following equation:

$$
J_{g}(x)=\Phi_{g, l}=-\frac{1}{3\left(\Sigma_{t, g}-\sum_{g^{\prime}=1}^{g^{\prime}=g} \Sigma_{g^{\prime} \rightarrow g, 1} \frac{\Phi_{g^{\prime}, l}}{\Phi_{g, l}}\right)} \frac{\partial \Phi_{g, 0}(x)}{\partial x}
$$

This relation is not very satisfactory since the current $\Phi_{g, l}$, that also appears at the denominator, is not completely defined, unlike the one-group case. Therefore, supplementary approximations must be applied to evaluate the transport-corrected cross section:

$$
\begin{equation*}
\text { Multi-group transport-corrected cross section: } \Sigma_{t, g}^{t r} \equiv \Sigma_{t, g}-\sum_{g^{\prime}=l}^{g^{\prime}=g} \Sigma_{g^{\prime} \rightarrow g, l} \frac{\Phi_{g^{\prime}, l}}{\Phi_{g, l}} \tag{9.25}
\end{equation*}
$$

Historically, several approximations have been proposed. The following hypothesis $\Sigma_{t, g}^{t r} \approx \Sigma_{t, g}-\Sigma_{g \rightarrow g, 1}$ is similar to considering that all the cross sections $\Sigma_{g^{\prime}} \neq g \rightarrow g, 1$ are zero and that all collisions are isotropic. This approximation is called the "diagonal transport approximation" since the scattering matrix is assumed to be diagonal. Another solution consists in setting $\Sigma_{t, g}^{t r} \approx \Sigma_{t, g}-$ $\sum_{g^{\prime \prime}=g}^{g^{\prime \prime}=G} \Sigma_{g \rightarrow g^{\prime \prime}, 1}$. This approximation employs a triangular slowing-down matrix for the first moment of the slowing-down cross section and thus conserves the anisotropy of neutrons scattered from group $g$. This approximation is called the "complete transport approximation". Finally, the last approach consists in setting $\Sigma_{t, g}^{t r} \approx \Sigma_{t, g}-\sum_{g^{\prime}=1}^{g^{\prime}=g} \Sigma_{g^{\prime} \rightarrow g, 1}$, thereby assuming that the current does not depend on energy, i.e. $\Phi_{g^{\prime}, 1} / \Phi_{g, 1} \equiv 1$. This hypothesis is called the "direct transport approximation". It should be pointed out that all these approximations aim at eliminating the current contribution in the transport-corrected cross section.

Studies have shown that these three approximations are satisfactory with respect to the exact transport equation for atoms with nuclear mass above 20 . For usual moderators such as water or carbon, the direct approximation works best. However, the true transport cross section (Eq. 9.25) should be employed as far as possible, by substituting the multi-group anisotropic current $\Phi_{g, l}$ computed by a multi-group transport code in a reference case and applied in a diffusion code for situations close to the latter.

## 9.4 $\boldsymbol{S P} \boldsymbol{P}_{\boldsymbol{n}}$ Method

In 1961, E. M. Gelbard proposed ${ }^{13}$ a new method called the $S P_{n}$ method for Simplified $P_{n}$, which implements the fact that neutrons have a massively monodirectional behavior. The general principle behind the method is to assume that the flux is locally $l D$, and thus the odd flux moments are replaced by vector quantities (which are called "currents") and the first derivatives of the odd moments are replaced by divergence operators (on the currents), while the first derivatives of the moments are substituted by gradients. In 1992, E. Larsen ${ }^{14}$ et al. showed that

[^192]

Ely Gelbard (1924-2002) Public domain

[^193]the $S P_{n}$ approach is the asymptotic limit of the transport equation. In 1993, G. Pomraning showed ${ }^{15}$ that it corresponds to the limit of the locally $l D$ transport equation. This limit indicates $l D$ transport locally with highly-forward scattering. Thus, instead of employing the spherical harmonics, Legendre polynomials are used to expand the flux on a truncated basis at order $n$ :
$$
\Phi(x, \mu)=\frac{1}{2} \sum_{l=0}^{l=n}(2 l+1) \Phi_{l}(x) P_{l}(\mu)
$$
with the flux moment defined as: $\Phi_{l}(x)=\int_{-1}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu$. The scattering cross section is itself expanded with Legendre polynomials for the cosine of the collision angle $\mu_{0}=\vec{\Omega} \cdot \vec{\Omega}^{\prime}$ :
$$
\Sigma_{s}\left(\vec{r}, \mu_{0}\right)=\frac{1}{2} \sum_{l=0}^{l=n}(2 l+1) \Sigma_{s, l}(\vec{r}) P_{l}\left(\mu_{0}\right)
$$

Some authors, such as (Blaquière 1962), consider that the scattering cross section can be simplified by expressing it as the summation of the product of Legendre polynomials of the cosine of the two angular directions $\mu=\vec{\Omega} \cdot \vec{x}$ and $\mu^{\prime}=\vec{\Omega}^{\prime} \cdot \vec{x}:$

$$
\Sigma_{s}\left(x, \mu_{0}\right) \approx \frac{1}{2} \sum_{l=0}^{l=n}(2 l+1) \Sigma_{s, l}(x) P_{l}(\mu) P_{l}\left(\mu^{\prime}\right)
$$



[^194]${ }^{15}$ G.C. Pomraning: Asymptotic and variational derivations of the simplified $P_{n}$ equations, Ann. Nucl. Energy, vol. 20, no. 9, pp. 623-637 (1993).

This approximation that omits some terms of the Legendre polynomials associated with the addition formula (Eq. 9.15) is not required in $1 D P_{n}$ theory. Indeed, the non-planar spherical harmonics moments of the scattering cross section simplify by the equation with the cancelling of orthogonal terms with the Legendre polynomials of the flux. Yet, it leads to the same linearized equations by simplifying the notations. Therefore, by injecting these expressions in the $1 D$ transport equation (Eq. 9.14), and similar to the $P_{n}$ technique, by choosing the $n+1$ moments of that equation wrt the first $n+1$ Legendre polynomials, the following $n+1$ equations are obtained:

$$
\begin{aligned}
& \frac{\partial}{\partial x} \int_{-1}^{+1} \mu \Phi(x, \mu) P_{l}(\mu) d \mu+\Sigma_{t}(x) \int_{-1}^{+1} \mu \Phi(x, \mu) P_{l}(\mu) d \mu \\
& =\frac{1}{2} \sum_{k=0}^{m}(2 k+1) \Sigma_{s, k} \Phi_{k}(x) \int_{-1}^{+1} P_{k}(\mu) P_{l}(\mu) d \mu+\underbrace{\int_{-1}^{+1} S(x, \mu) P_{l}(\mu) d \mu}_{s_{l}(x)} \quad \text { for } l=0, n
\end{aligned}
$$

This equation can be written as:

$$
\begin{aligned}
& \sum_{k=1}^{n} \frac{\partial}{\partial x} \frac{2 k+1}{2} \Phi_{k}(x) \int_{-1}^{+1} \mu P_{k}(\mu) P_{l}(\mu) d \mu+\Sigma_{t}(x) \Phi_{l}(x) \\
& \quad=\sum_{k=0}^{m} \Sigma_{s, k} \Phi_{k}(x) \delta_{k l}+S_{l}(x) \quad \text { for } \quad l=0, n
\end{aligned}
$$

Using the recurrence properties of the Legendre polynomials, the integral term is computed as:

$$
\int_{-1}^{+1} \mu P_{k}(\mu) P_{l}(\mu) d \mu=\int_{-1}^{+1}\left[\frac{k+1}{2 k+1} P_{k+1}(\mu)+\frac{k}{2 k+1} P_{k-1}(\mu)\right] P_{l}(\mu) d \mu
$$

Thus:

$$
\begin{aligned}
& \sum_{k=1}^{n} \frac{\partial}{\partial x} \frac{2 k+1}{2} \Phi_{k}(x) \int_{-1}^{+1} \mu P_{k}(\mu) P_{l}(\mu) d \mu \\
& \quad=\frac{l+1}{2 l+1} \Phi_{k+1}(x) \delta_{(k+1), l}+\frac{l}{2 l+1} \Phi_{k-1}(x) \delta_{(k-1), l}
\end{aligned}
$$

Only one of these two terms can be non-zero. Usual practice is to introduce a current vector for the odd values of $l: \overrightarrow{\Phi_{2 l+1}}=\Phi_{2 l+1} \vec{x}$, and by expressing the previous equations for the three space directions, a system of differential equations is reached, for both scalar and vector quantities, as (by dropping the space dependence):
$S P_{n}$ equations:

$$
\begin{cases}\left(\Sigma_{t}-\Sigma_{s, 0}\right) \Phi_{0}+\operatorname{div} \overrightarrow{\Phi_{1}} & =S_{0} \\ \frac{1}{3} \overrightarrow{\operatorname{grad} \Phi_{0}+\left(\Sigma_{t}-\Sigma_{s, 1}\right) \overrightarrow{\Phi_{1}}+\frac{2}{3} \overrightarrow{\operatorname{grad}} \Phi_{2}} & =S_{1}  \tag{9.26}\\ \frac{2}{5} \operatorname{div} \overrightarrow{\Phi_{1}}+\left(\Sigma_{t}-\Sigma_{s, 2}\right) \Phi_{2}+\frac{3}{5} \operatorname{div} \overrightarrow{\Phi_{3}} & =S_{2} \\ \vdots & \\ \frac{2 l}{4 l+1} \operatorname{div} \overrightarrow{\Phi_{2 l-1}}+\left(\Sigma_{t}-\Sigma_{s, 2 l}\right) \Phi_{2 l}+\frac{2 l+1}{4 l+1} \operatorname{div} \overrightarrow{\Phi_{2 l+1}} & =S_{2 l} \\ \frac{2 l+1}{4 l+3} \overrightarrow{\operatorname{grad}} \Phi_{2 l}+\left(\Sigma_{t}-\Sigma_{s, 2 l+1}\right) \overrightarrow{\Phi_{2 l+1}}+\frac{2 l+2}{4 l+3} \overrightarrow{g r a d} \Phi_{2 l+2} & =S_{2 l+1} \\ \vdots & \\ \frac{n}{2 n+1} \overrightarrow{\operatorname{grad} \Phi_{n-1}+\left(\Sigma_{t}-\Sigma_{s, n}\right) \overrightarrow{\Phi_{n}}} & =S_{n}\end{cases}
$$

These equations are very similar to the diffusion equation with the flux moment $\Phi_{2 l}$ and its associated current moment $\overrightarrow{\Phi_{2 l+1}}$. The $S P_{n}$ approach is hence equivalent to solving $(n+1) / 2$ diffusion problems. It is easy to show that $S P_{1}$ is equivalent to the diffusion problem. This vector approach is not founded on the flux expansion on spherical harmonics but stems from a variational approach using $P_{l}(\vec{\Omega} \cdot \overrightarrow{\text { grad })})$ test functions which were introduced by G. Pomraning ${ }^{16}$ :

[^195]$$
\Phi(\vec{r}, \vec{\Omega})=\sum_{l=0}^{L} \frac{2 l+1}{4 \pi} P_{l}(\vec{\Omega} \cdot \overrightarrow{g r a d})\left[\Phi_{l}(\vec{r})\right]
$$

These test functions are in fact operators that deal with a space function, and which are an extension of the Legendre polynomials in which the argument is replaced by $\vec{\Omega} \cdot \overrightarrow{g r a d}$, i.e. ${ }^{17}$ :

$$
\begin{aligned}
& P_{0}(\vec{\Omega} \cdot \overrightarrow{g r a d})[]=1, P_{1}(\vec{\Omega} \cdot \overrightarrow{g r a d})[]=\vec{\Omega} \cdot \overrightarrow{g r a d}[], P_{2}(\vec{\Omega} \cdot \overrightarrow{g r a d})[] \\
&=\frac{1}{2}\left(3(\vec{\Omega} \cdot \overrightarrow{g r a d})^{2}-\Delta\right)[], \\
& P_{3}(\vec{\Omega} \cdot \overrightarrow{g r a d})[]=\frac{1}{2} \vec{\Omega} \cdot \overrightarrow{g r a d}\left(5(\vec{\Omega} \cdot \overrightarrow{g r a d})^{2}-3 \Delta\right)[], \cdots
\end{aligned}
$$

These functions form an incomplete orthonormal basis for which the orthogonality principle is expressed as:

$$
\int_{4 \pi} d \vec{\Omega} P_{l}(\vec{\Omega} \cdot \overrightarrow{g r a d})\left[P_{l^{\prime}}(\vec{\Omega} \cdot \overrightarrow{g r a d})[\Phi(\vec{r})]\right]=\frac{4 \pi}{2 l+1} \delta_{l, l^{\prime}} \Delta^{l}[\Phi(\vec{r})]
$$

where the generalized Laplace operator is written as: $\Delta^{l}[\Phi(\vec{r})] \equiv \Delta^{l-1}[\Delta[\Phi(\vec{r})]]$ and $\Delta[] \equiv \overrightarrow{\operatorname{grad}} \cdot \overrightarrow{g r a d}[]$

It should be noted that the function $\Phi(\vec{r})$ must de differentiable $2 L$ times. Once these operators are defined, the flux solution expressed on this basis of test functions

[^196](and the source terms with the same expansion) is injected in the system of equations and multiplied successively by the $P_{l}(\vec{\Omega} . \overrightarrow{\text { grad })})$ operators. Afterwards, integration over the unit sphere $(4 \pi)$ is carried out to ensure the orthogonality condition is satisfied via a projection technique on the usual basis. The system of equations given by Eq. (9.26) is thus obtained. Hebert developed a variational approach for the method by constructing a functional for the even and odd flux, where Eq. (9.26) is deduced by the stationary property of the mixed dual functional.

Although increasing the order of the method does not converge towards the exact solution, it has been observed that $S P_{3}$ or $S P_{5}$ brought numerical improvements wrt the exact solution or a best-estimate solution computed by the transport method compared to the diffusion approximation. Thus, in the 1990's, with the increasing computational power, these methods were appreciated for dealing with $3 D$ geometries. Nonetheless, the $S P_{n}$ method remains a satisfactory preconditioner of the $P_{n}$ method.

### 9.5 Interfaces Between Different Media

The differential equations of the $P_{n}$ problem (Eq. 9.22) or even the $S P_{n}$ method can be solved using the following flux expansion:

$$
\Phi(x, \mu)=\frac{1}{2} \sum_{l=0}^{l=n}(2 l+1) \Phi_{l}^{k}(x) P_{l}(\mu) \quad \text { with: } \quad \Phi_{l}^{k}(x)=\varphi_{l}\left(\lambda_{k}\right) e^{-\frac{\varepsilon_{l x}}{\lambda_{k}}}
$$

Expressing the exponential coefficient in terms of $\Sigma_{t} x$ is equivalent to working with mean free paths in the space dimension, and $\lambda_{k}$ is a dimensionless number defined as the number of free paths. The general solution to the differential system is then written as the sum of the particular solution of the equation with a source and a general solution for the equation without source:

$$
\Phi(x, \mu)=\frac{S_{0}}{2\left(\Sigma_{t}-\Sigma_{s, 0}\right)}+\sum_{k=0}^{k=n} \Psi_{k} \Phi_{k}(x)
$$

Since $\partial \Phi_{l}^{k}(x) / \partial x=-\Sigma_{t} \Phi_{l}^{k}(x) / \lambda_{k}, \lambda_{k}$ satisfies the linear system of equations obtained when the flux solution $\Phi_{l}^{k}(x)$ is injected in Eq. (9.22):

$$
\left\{\begin{array}{c}
\lambda \frac{\left(\Sigma_{t}-\Sigma_{s, 0}\right)}{\Sigma_{t}} \varphi_{0}-\varphi_{1}=0 \\
\vdots \\
-l \varphi_{l-1}+(2 l+1) \lambda \frac{\left(\Sigma_{t}-\Sigma_{s, l}\right)}{\Sigma_{t}} \varphi_{l}-(l+1) \varphi_{l+1}=0 \\
\vdots \\
-(n-1) \varphi_{n-2}+(2 n-1) \lambda \frac{\left(\Sigma_{t}-\Sigma_{s, n-1}\right)}{\Sigma_{t}} \varphi_{n-1}-n \varphi_{n}=0 \\
\\
\quad-n \varphi_{n-1}+(2 n+1) \lambda \frac{\left(\Sigma_{t}-\Sigma_{s, n}\right)}{\Sigma_{t}} \varphi_{n}=0
\end{array}\right.
$$

This equation system has a set of non-trivial (non-zero) solutions $\varphi_{l=0, n}$ only if the determinant of the corresponding matrix is zero: $\operatorname{det} A\left(n, \lambda, \Sigma_{t}, \Sigma_{s}, l=0, n\right)=0$. The latter is a $n+1$-degree polynomial in $\lambda$ for which it can be easily shown that $\lambda=0$ is a trivial solution if $n+1$ is odd (i.e. $n$ is even) since $\lambda$ appears only in the diagonal terms of the matrix. The flux behavior is non-physical with a constant component in $x$, which is why, in practice, an even expansion is never used in the $P_{n}$ method. If $n$ is odd, the determinant is polynomial with a bi-quadratic term in $\lambda^{2}$ and the solutions in $\lambda_{k}$ are coupled as pairs of positive and negative values $\pm \lambda_{k}$. In the general case of an interface between two media, $n+1$ closure equations are required to calculate the $\psi_{k=0, n}$ coefficients. Assuming that the flux is finite at infinity for infinite media, it can be simply established that the $\psi_{k}$ coefficients for positive exponential terms are zero. If the $\lambda$ coefficients are the roots of the determinant, the equation is tightly coupled. Thus, an arbitrary value of $\varphi_{n}$ is chosen to calculate the $\varphi_{l=0, n-1}$ terms successively (or in matrix form). The particular case of a homogeneous medium where the total cross section is constant and the scattering cross section is linearly anisotropic (only $\sum_{s, 0}$ and $\sum_{s, 1}$ are non-zero) is often computed in practical cases since it allows a solution for the following system:

$$
\left\{\begin{array}{l}
\lambda \frac{\left(\Sigma_{t}-\Sigma_{s, 0}\right)}{\Sigma_{t}} \varphi_{0}-\varphi_{1}=0 \\
-\varphi_{l-1}+3 \lambda \frac{\left(\Sigma_{t}-\Sigma_{s, l}\right)}{\Sigma_{t}} \varphi_{l}-2 \varphi_{l+1}=0 \\
\vdots \\
-l \varphi_{l-1}+(2 l+1) \lambda \varphi_{l}-(l+1) \varphi_{l+1}=0 \\
\vdots \\
-(n-1) \varphi_{n-2}+(2 n-1) \lambda \varphi_{n-1}-n \varphi_{n}=0 \\
-n \varphi_{n-1}+(2 n+1) \lambda \varphi_{n}=0
\end{array}\right.
$$

Except for the first two equations, it can be observed that the $\varphi_{l=2, n-1}$ terms satisfy the recurrence relations of the Legendre polynomials. Jahnke and Emde (Jahnke and Emde 1945) noted that there exists another polynomial series $W_{l}(\lambda)$ of degree $l$ in $\lambda$, and defined as:

$$
W_{l}(\lambda)=\frac{1}{2} \int_{-1}^{+1} \frac{P_{l+1}(\lambda)-P_{l+1}(\mu)}{\lambda-\mu} d \mu
$$

that satisfies the same recurrence relation as the Legendre polynomials with a shift of 1 for the indices:

$$
(l+1) W_{l}(\lambda)-(2 l+1) \lambda W_{l-1}(\lambda)+l W_{l-2}(\lambda)
$$

A study of these polynomials $\left(W_{0}(\lambda)=1, W_{1}(\lambda)=3 \lambda / 2, W_{2}(\lambda)=5 \lambda^{2} / 2-2 / 3\right.$, etc.) showed that they are not proportional to the Legendre polynomials (except the first two), thereby leading to their use for calculating the $\varphi_{l=2, n-1}(\lambda)$ coefficients by fixing (Weinberg and Wigner 1958, p. 249):

$$
\varphi_{l=2, n-1}(\lambda)=A P_{l}(\lambda)-B W_{l-1}(\lambda)
$$

From the respective recurrence relations, it is easily shown that the coefficients $A$ and $B$ are constant for any $l \geq 2$. Given that the equations for $\varphi_{l}$ are homogeneous, there is a degree of freedom such that $A$ is arbitrarily chosen as $A=1$. The coefficient $B$ is obtained by cancelling the $n+1^{\text {th }}$ flux moment $\varphi_{n+1}$, i.e.:

$$
B=\frac{W_{n}(\lambda)}{P_{n+1}(\lambda)}
$$

The continuity of the different flux moments between two media allows the establishing of a linear system of equations given that the flux is expanded at the same order on both sides of the interface.

### 9.6 Spherical Harmonics Method

(Stamm'ler and Abbate 1983, p. 142; Ferziger and Zweifel 1966, p. 132; Meghreblian and Holmes 1960, p. 338).

### 9.6.1 Principle

The use of Legendre polynomials is particularly well suited to one-dimensional cases. In more general $3 D$ cases, the spherical harmonics cannot be projected in the plane geometry. Let us consider the complete flux expression:

$$
\Phi(\vec{r}, \vec{\Omega})=\sum_{l=0}^{l=+\infty} \sum_{m=-1}^{m=+1} \Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})
$$

The spherical harmonics are widely employed in quantum physics and in field theory ${ }^{18}$ (description of wave functions in spherical coordinates). Thus, the equations are written with the analogy to these fields with the principal quantum number $(l)$ and the secondary one $(m)$. The normalized (to unity) spherical harmonics are expressed as:

$$
\begin{cases}Y_{l}^{m}(\vec{\Omega})=(-1)^{m} \sqrt{\frac{2 l+1}{4 \pi}} \sqrt{\frac{(l-m)!}{(l-m)!}} P_{l}^{m}(\mu) e^{i m \varphi} & \text { for } \quad m>0 \\ Y_{l}^{m}(\vec{\Omega})=(-1)^{-m} Y_{l}^{m}(\vec{\Omega}) & \text { for } \\ Y_{0}^{0}(\vec{\Omega})=m<0 \\ Y_{0}^{0}(\vec{\Omega})=\frac{1}{\sqrt{4 \pi}} & \end{cases}
$$

The flux, expressed in spherical coordinates, is written as:

$$
\Delta \Phi(r, \theta, \varphi)=\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial \Phi(r, \theta, \varphi)}{\partial r}\right)+\frac{1}{r^{2}} \underbrace{\left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial \Phi(r, \theta, \varphi)}{\partial \theta}\right)+\frac{1}{\sin ^{2} \theta} \frac{\partial^{2} \Phi(r, \theta, \varphi)}{\partial \varphi^{2}}\right)}_{\Delta_{s} \Phi}
$$

The angular part of the Laplace operator is called the self-adjoint LaplaceBeltrami ${ }^{19}$ operator $\Delta_{s} \Phi$ (on the unit sphere $S$ ), for which the spherical harmonics are the eigenfunctions of:

$$
\Delta_{s} Y_{l}^{m}+l(l+1) Y_{l}^{m}=0
$$

For $l \geq 0$ and $-l \leq m \leq+l$, the spherical harmonics form an orthogonal basis for $L^{2}(S)$. Since the spherical harmonics $Y_{l}^{m}(\vec{\Omega})$ are complex numbers while the flux are real values, the components $\Phi_{l}^{m}$ and $\Phi_{l}^{-m}$ are related such that the combination of two spherical harmonics of different signs is a real number:

$$
\Phi_{l}^{-m}(\vec{r}) Y_{l}^{-m}(\vec{\Omega})+\Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})=\overline{\Phi_{l}^{-m}(\vec{r}) Y_{l}^{-m}(\vec{\Omega})+\Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})}
$$

i.e. by conjugating term by term (the conjugate of a product is the product of conjugates):

[^197]$\Phi_{l}^{-m}(\vec{r}) Y_{l}^{-m}(\vec{\Omega})+\Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})=\overline{\Phi_{l}^{-m}}(\vec{r})(-1)^{-m} Y_{l}^{m}(\vec{\Omega})+\overline{\Phi_{l}^{m}}(\vec{r})(-1)^{m} Y_{l}^{-m}(\vec{\Omega})$
As the spherical harmonics form a complete basis, the coefficients of a given harmonic can be identified (this is equivalent to using the orthogonality property), such as:
\[

\left\{$$
\begin{array}{l}
\Phi_{l}^{-m}=(-1)^{m} \overline{\Phi_{l}^{m}} \\
\boldsymbol{\Phi}_{l}^{m}=(-1)^{-m} \overline{\boldsymbol{\Phi}_{l}^{-m}}
\end{array}
$$\right.
\]

This result implies that:

$$
\begin{cases}\Phi_{l}^{-m}+\Phi_{l}^{+m} & \text { is real if } m \text { is even } \\ \Phi_{l}^{-m}-\Phi_{l}^{+m} & \text { is purely imaginary if } m \text { is odd }\end{cases}
$$



Eugenio Beltrami (Public domain)

This is why some authors ${ }^{20}$ prefer a flux expansion using non-normalized spherical harmonics:

$$
\Phi(\vec{r}, \vec{\Omega})=\sum_{l=0}^{l=+\infty} \sum_{m=0}^{l} \frac{2 l+1}{4 \pi} P_{l}^{m}(\mu)\left[\psi_{l}^{m}(\vec{r}) \cos (m \varphi)+\phi_{l}^{m} \sin (m \varphi)\right]
$$

with:

$$
\begin{cases}(-1)^{m} \sqrt{\frac{2 l+1}{4 \pi}} \sqrt{\frac{(l-m)!}{(l-m)!}} \psi_{l}^{m}= \begin{cases}\frac{1}{2}\left(\Phi_{l}^{+m}+\Phi_{l}^{-m}\right) & \text { which is real when } m \text { is even } \\ \frac{1}{2}\left(\Phi_{l}^{+m}-\Phi_{l}^{-m}\right) & \text { which is real when } m \text { is odd }\end{cases} \\ (-1)^{m} \sqrt{\frac{2 l+1}{4 \pi}} \sqrt{\frac{(l-m)!}{(l-m)!}} \phi_{l}^{m}= \begin{cases}\frac{1}{2 i}\left(\Phi_{l}^{+m}+\Phi_{l}^{-m}\right) & \text { which is real when } m \text { is even } \\ \frac{1}{2 i}\left(\Phi_{l}^{+m}-\Phi_{l}^{-m}\right) & \text { which is real when } m \text { is odd }\end{cases} \end{cases}
$$

It can be noted that the number of flux moments to calculate is the same in both approaches. The scattering cross section is written in terms of spherical harmonics using the addition theorem:

$$
\begin{aligned}
P_{n}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right) & \left.=\frac{4 \pi}{2 n+1} \sum_{m=-n}^{m=+n} Y_{n}^{m}(\vec{\Omega}) \overline{Y_{n}^{m}\left(\overrightarrow{\Omega^{\prime}}\right.}\right) \\
\Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) & =\sum_{l=0}^{l=+\infty} \frac{2 l+1}{4 \pi} \Sigma_{s, l}(\vec{r}) P_{l}\left(\mu_{0}\right) \\
& =\sum_{l=0}^{l=+\infty} \Sigma_{s, l}(\vec{r}) \sum_{m=-l}^{m=+l} Y_{l}^{m}(\vec{\Omega}) \overline{Y_{l}^{m}\left(\overrightarrow{\Omega^{\prime}}\right)}
\end{aligned}
$$

The orthogonality property of spherical harmonics results in the Hermitian scalar product of a harmonic with the conjugate of another harmonic:

$$
\int_{4 \pi} Y_{l}^{m}(\vec{\Omega}) \overline{Y_{l^{\prime}}^{m^{\prime}}}(\vec{\Omega}) d \vec{\Omega}=\delta_{l l^{\prime}} \delta_{m m^{\prime}}
$$

and the projection of the differential scattering cross section on a given harmonic is obtained:

[^198]$$
\int_{\vec{\Omega}} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}=\Sigma_{s, m} Y_{l}^{m}(\vec{\Omega})
$$

These various results lead to the calculation of the scattering operator:

$$
\left.\begin{array}{r}
\int_{\vec{\Omega},} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}=\int_{\vec{\Omega}}\left(\sum_{l=0}^{l=+\infty} \Sigma_{s, l}(\vec{r}) \sum_{m=-l}^{m=+l} Y_{l}^{m}(\vec{\Omega})\right.
\end{array} Y_{l}^{m}\left(\vec{\Omega}^{\prime}\right)\right)
$$

The above resulting equation simplifies the integro-differential transport equation as follows:

$$
\begin{align*}
\vec{\Omega} . & \sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} \overrightarrow{\operatorname{grad}} \Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})+\Sigma_{t} \sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} \Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega}) \\
= & \sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} \Sigma_{s, l}(\vec{r}) \Phi_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})+\sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} S_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega}) \tag{9.27}
\end{align*}
$$

If the fission source is assumed isotropic, thus:

$$
S(\vec{r}, \vec{\Omega})=\frac{1}{4 \pi} \frac{v \Sigma_{f}(\vec{r})}{k_{e f f}}
$$

which is expressed under the form: $S(\vec{r}, \vec{\Omega})=\frac{1}{\sqrt{4 \pi}} \frac{v \Sigma_{f}(\vec{r})}{k_{\text {eff }}} Y_{0}^{0}(\vec{\Omega})=S_{0}^{0}(\vec{r}) Y_{0}^{0}(\vec{\Omega})$ to simplify the angular integration of flux moments. Equation (9.27) includes the products $\vec{\Omega} \cdot Y_{l}^{m}(\vec{\Omega})$. By noting that:

$$
\vec{\Omega}=\binom{\sin \theta \cos \varphi=\frac{\sin \theta}{2}\left(e^{i \varphi}+e^{-i \varphi}\right)}{\sin \theta \cos \varphi=\frac{\sin \theta}{2 i}\left(e^{i \varphi}+e^{-i \varphi}\right)}=\left(\begin{array}{c}
\sqrt{\frac{2 \pi}{3}\left(Y_{1}^{-1}-Y_{1}^{1}\right)} \\
\cos \theta \\
\left.\sqrt{\frac{2 \pi}{3}\left(Y_{1}^{-1}+Y_{1}^{1}\right.}\right) \\
\sqrt{\frac{4 \pi}{3} Y_{1}^{0}}
\end{array}\right)
$$

The recurrence relations for spherical harmonics can be employed (while dropping the angular dependence $\vec{\Omega}$ for notations):

$$
\begin{aligned}
& \cos \theta Y_{l}^{m}=\underbrace{\sqrt{\frac{(l+m)(l-m)}{(2 l-1)(2 l+1)}}}_{a_{l-1}^{m}} Y_{l-1}^{m}+\underbrace{\sqrt{\frac{(l+1+m)(l+1-m)}{(2 l+1)(2 l-3)}}}_{a_{l+1}^{m}} Y_{l+1}^{m} \\
& \equiv a_{l-1}^{m} Y_{l-1}^{m}+a_{l+1}^{m} Y_{l+1}^{m} \\
& \begin{aligned}
\sin \theta e^{i \varphi} Y_{l}^{m} & =\underbrace{\sqrt{\frac{(l-m-1)(l-m)}{(2 l-1)(2 l+1)}}}_{b_{l-1}^{m+1}} Y_{l-1}^{m+1}-\underbrace{\sqrt{\frac{(l+1+m)(l+2+m)}{(2 l+1)(2 l+3)}}}_{b_{l+1}^{m+1}} Y_{l+1}^{m+1} \\
& \equiv b_{l-1}^{m+1} Y_{l-1}^{m+1}-b_{l+1}^{m+1} Y_{l+1}^{m+1}
\end{aligned} \\
& \sin \theta e^{-i \varphi} Y_{l}^{m}=-\underbrace{l-1}_{\substack{c_{l-1}^{m-1} \\
\sqrt{\frac{(l+m-1)(l+m)}{(2 l-1)(2 l+1)}}}}{ }_{l-1}^{m-1}+\underbrace{\sqrt{\frac{(l-m+1)(l-m+2)}{(2 l+1)(2 l+3)}}}_{\substack{c_{l+1}^{m-1}}} Y_{l+1}^{m-1} \\
& \equiv-c_{l-1}^{m-1} Y_{l-1}^{m-1}+c_{l+1}^{m-1} Y_{l+1}^{m-1}
\end{aligned}
$$

From the properties of conjugate terms, the recurrence laws for the harmonics with negative $m$ coefficients are deduced as:

$$
\begin{aligned}
\cos \theta Y_{l}^{-m} & =\cos \theta(-1)^{-m}{\overline{Y_{l}^{m}}=(-1)^{-m}\left[a_{l-1}^{m}(-1)^{-m} Y_{l-1}^{-m}+a_{l+1}^{m}(-1)^{-m} Y_{l+1}^{-m}\right]}=a_{l-1}^{m} Y_{l-1}^{-m}+a_{l+1}^{m} Y_{l+1}^{-m}
\end{aligned}
$$

Therefore: $a_{l-1}^{-m}=a_{l-1}^{m}$ and $a_{l+1}^{-m}=a_{l+1}^{m}$
$\left\{\begin{array}{l}\sin \theta \overline{e^{-i \varphi} Y_{l}^{m}}=\sin \theta e^{-i \varphi}(-1)^{m} Y_{l}^{-m}=-c_{l-1}^{m-1} \overline{Y_{l-1}^{m-1}}+c_{l+1}^{m-1} \overline{Y_{l+1}^{m-1}} \\ \sin \theta e^{-i \varphi} Y_{l}^{-m}=c_{l-1}^{m-1} Y_{l-1}^{-(m-1)}-c_{l+1}^{m-1} Y_{l+1}^{-(m-1)} \equiv b_{l-1}^{-(m-1)} Y_{l-1}^{-(m-1)}-b_{l+1}^{-(m-1)} Y_{l+1}^{-(m-1)}\end{array}\right.$
Hence: $b_{l-1}^{-(m-1)}=c_{l-1}^{m-1}$ and $b_{l+1}^{-(m-1)}=c_{l+1}^{m-1}$
$\left\{\begin{array}{l}\sin \theta \overline{e^{i \varphi} Y_{l}^{m}}=\sin \theta e^{-i \varphi}(-1)^{m} Y_{l}^{-m}=b_{l-1}^{m+1} \overline{Y_{l-1}^{m+1}}-b_{l+1}^{m+1} \overline{Y_{l+1}^{m+1}} \\ \sin \theta e^{-i \varphi} Y_{l}^{-m}=-b_{l-1}^{m+1} Y_{l-1}^{-(m+1)}+b_{l+1}^{m+1} Y_{l+1}^{-(m+1)} \equiv-c_{l-1}^{(m+1)} Y_{l-1}^{-(m+1)}+c_{l+1}^{-(m+1)} Y_{l+1}^{-(m+1)}\end{array}\right.$
Thus: $c_{l-1}^{-(m+1)}=b_{l-1}^{m+1}$ and $c_{l+1}^{-(m+1)}=b_{l+1}^{m+1}$.
The formulae for the coefficients $b$ and $c$ are interchanged for negative flux moments. Substituting these expressions in the integro-differential equations eventually leads to:

$$
\begin{aligned}
& \sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} \frac{\partial \Phi_{l}^{m}}{\partial x} \frac{1}{2}\left(b_{l-1}^{m+1} Y_{l-1}^{m+1}-b_{l+1}^{m+1} Y_{l+1}^{m+1}-c_{l-1}^{m-1} Y_{l-1}^{m-1}+c_{l+1}^{m-1} Y_{l+1}^{m-1}\right) \\
& +\sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} \frac{\partial \Phi_{l}^{m}}{\partial y} \frac{1}{2 i}\left(b_{l-1}^{m+1} Y_{l-1}^{m+1}-b_{l+1}^{m+1} Y_{l+1}^{m+1}+c_{l-1}^{m-1} Y_{l-1}^{m-1}-c_{l+1}^{m-1} Y_{l+1}^{m-1}\right) \\
& +\sum_{l=0}^{l=+\infty} \sum_{m=-l}^{m=+l} \frac{\partial \Phi_{l}^{m}}{\partial z}\left[a_{l-1}^{m} Y_{l}^{m}+a_{l+1}^{m} Y_{l+1}^{m}\right]+\Sigma_{t} \sum_{l=0}^{l=+\infty m=+l} \sum_{m=-l} \Phi_{l}^{m} Y_{l}^{m}=\sum_{l=0}^{l=+\infty m=+l} \sum_{m=-l} \Phi_{l}^{m} \Sigma_{s, l} Y_{l}^{m}+\sum_{l=0}^{l=+\infty m=+l} \sum_{m=-l} S_{l}^{m} Y_{l}^{m}
\end{aligned}
$$

As seen previously, it is wiser to group harmonics of opposite signs so as to deal with real values. By separating the contribution for $m=0$ that can be calculated directly, the three successive leakage terms (streaming) are:

Term for $x$ :

$$
\begin{aligned}
& \sqrt{\frac{2 \pi}{3}}\left(Y_{1}^{-1}-Y_{1}^{1}\right) \frac{\partial \Phi_{0}^{0}}{\partial x} Y_{0}^{0}+\frac{1}{2} \sum_{l=1}^{l=+\infty} \sum_{m=l}^{m=+l} \frac{\partial \Phi_{l}^{m}}{\partial x}\left(b_{l-1}^{m+1} Y_{l-1}^{m+1}-b_{l+1}^{m+1} Y_{l+1}^{m+1}\right. \\
& \left.-c_{l-1}^{m-1} Y_{l-1}^{m-1}+c_{l+1}^{m-1} Y_{l+1}^{m-1}\right)+\sum_{l=1}^{l=+\infty} \sqrt{\frac{2 \pi}{3}}\left(Y_{1}^{-1}-Y_{1}^{-1}\right) \frac{\partial \Phi_{l}^{0}}{\partial x} \\
& +\frac{1}{2} \sum_{l=1}^{l=+\infty} \sum_{m=l}^{m=+l} \frac{\partial \Phi_{l}^{-m}}{\partial x}\left(c_{l-1}^{m-1} Y_{l-1}^{-(m-1)}-c_{l+1}^{m-1} Y_{l+1}^{-(m-1)}\right. \\
& \left.-b_{l-1}^{m+1} Y_{l-1}^{-(m+1)}+b_{l+1}^{m+1} Y_{l+1}^{-(m+1)}\right)
\end{aligned}
$$

Term for $y$ :

$$
\begin{aligned}
& i \sqrt{\frac{2 \pi}{3}}\left(Y_{1}^{-1}+Y_{1}^{1}\right) \frac{\partial \Phi_{0}^{0}}{\partial x} Y_{0}^{0}+\frac{1}{2 i} \sum_{l=1}^{l=+\infty m=+l} \sum_{m=l}^{m} \frac{\partial \Phi_{l}^{m}}{\partial y}\left(b_{l-1}^{m+1} Y_{l-1}^{m+1}-b_{l+1}^{m+1} Y_{l+1}^{m+1}\right. \\
& \left.+c_{l-1}^{m-1} Y_{l-1}^{m-1}-c_{l+1}^{m-1} Y_{l+1}^{m+1}\right)+\sum_{l=1}^{l=+\infty} \sqrt{\frac{2 \pi}{3}}\left(Y_{1}^{-1}+Y_{1}^{1}\right) \frac{\partial \Phi_{l}^{0}}{\partial x} \\
& +\frac{1}{2 i} \sum_{l=1}^{l=+\infty m=+l} \sum_{m=l} \frac{\partial \Phi_{l}^{-m}}{\partial y}\left(c_{l-1}^{m-1} Y_{l-1}^{-(m-1)}-c_{l+1}^{m-1} Y_{l+1}^{-(m-1)}+b_{l-1}^{m+1} Y_{l-1}^{-(m+1)}\right. \\
& \left.\quad-b_{l+1}^{m+1} Y_{l+1}^{-(m+1)}\right)
\end{aligned}
$$

Term for $z$ :

$$
\begin{align*}
& \sqrt{\frac{4 \pi}{3}} Y_{1}^{0} \frac{\partial \Phi_{0}^{0}}{\partial z} Y_{0}^{0}+\sum_{l=1}^{l=+\infty m=+l} \sum_{m=l}^{m} a_{l-1}^{m}\left(\frac{\partial \Phi_{l}^{m}}{\partial z} Y_{l-1}^{m}+\frac{\partial \Phi_{l}^{-m}}{\partial z} Y_{l-1}^{-m}\right) \\
& +a_{l+1}^{m}\left(\frac{\partial \Phi_{l}^{m}}{\partial z} Y_{l+1}^{m}+\frac{\partial \Phi_{l}^{-m}}{\partial z} Y_{l+1}^{-m}\right)+\sum_{l=1}^{l=+\infty} \sqrt{\frac{4 \pi}{3}} Y_{1}^{0} \frac{\partial \Phi_{l}^{0}}{\partial z} \tag{9.28}
\end{align*}
$$

Injecting these expressions in the integro-differential equation and by limiting the expansion to order $n$, the general recurrence relation for the flux moments is reached by identifying term-wise the coefficients of $Y_{l}^{m}$ and $Y_{l}^{-m}$ (for $l \geq 2$ ):

$$
\left\{\begin{array}{l}
a_{l}^{m}\left(\frac{\partial \Phi_{l+1}^{m}}{\partial z}+\frac{\partial \Phi_{l-1}^{m}}{\partial z}\right)+\frac{1}{2}\left[\left(\frac{\partial \Phi_{l+1}^{m-1}}{\partial x}-\frac{\partial \Phi_{l-1}^{m-1}}{\partial x}\right) b_{l}^{m}+\left(\frac{\partial \Phi_{l+1}^{m+1}}{\partial x}+\frac{\partial \Phi_{l-1}^{m+1}}{\partial x}\right) c_{l}^{m}\right] \\
\frac{1}{2 i}\left[\left(\frac{\partial \Phi_{l+1}^{m-1}}{\partial y}-\frac{\partial \Phi_{l-1}^{m-1}}{\partial y}\right) b_{l}^{m}+\left(\frac{\partial \Phi_{l+1}^{m+1}}{\partial y}-\frac{\partial \Phi_{l-1}^{m+1}}{\partial y}\right) c_{l}^{m}\right]+\Sigma_{t} \Phi_{l}^{m}=\Sigma_{s, l} \Phi_{l}^{m}+S_{l}^{m} \\
a_{l}^{m}\left(\frac{\partial \Phi_{l+1}^{-m}}{\partial z}+\frac{\partial \Phi_{l-1}^{-m}}{\partial z}\right)+\frac{1}{2}\left[\left(\frac{\partial \Phi_{l+1}^{-(m+1)}}{\partial x}-\frac{\partial \Phi_{l-1}^{-(m+1)}}{\partial x}\right) c_{l}^{m}+\left(\frac{\partial \Phi_{l+1}^{-(m-1)}}{\partial x}+\frac{\partial \Phi_{l-1}^{-(m-1)}}{\partial x}\right) b_{l}^{m}\right] \\
\frac{1}{2 i}\left[\left(\frac{\partial \Phi_{l+1}^{-(m+1)}}{\partial y}-\frac{\partial \Phi_{l-1}^{-(m+1)}}{\partial y}\right) c_{l}^{m}+\left(\frac{\partial \Phi_{l+1}^{-(m-1)}}{\partial y}-\frac{\partial \Phi_{l-1}^{-(m-1)}}{\partial y}\right) b_{l}^{m}\right]+\Sigma_{t} \Phi_{l}^{-m}=\Sigma_{s, l} \Phi_{l}^{-m}+S_{l}^{-m}
\end{array}\right.
$$

These two equations are summed term-wise and using the real and imaginary parts of the flux, $\psi_{l}^{m}$ and $\varphi_{l}^{m}$ respectively, that are related to the flux moments by:

$$
\left\{\begin{array}{llll}
m \text { even } & : & \Phi_{l}^{+m}+\Phi_{l}^{-m}=2 \psi_{l}^{m} & \Phi_{l}^{+m}-\Phi_{l}^{-m}=2 i \varphi_{l}^{m} \\
m \text { odd } & : & \Phi_{l}^{+m}+\Phi_{l}^{-m}=2 i \varphi_{l}^{m} & \Phi_{l}^{+m}-\Phi_{l}^{-m}=2 \psi_{l}^{m}
\end{array}\right.
$$

a real terms system of two differential equations, one for $m$ even, the other for $m$ $o d d$, is obtained which after simplification by $i$ (left in the formulation to clarify the reasoning by carefully noting that $1 / i=-i$ ):

$$
\left\{\begin{array}{l}
2 a_{l}^{m}\left(\frac{\partial \psi_{l+1}^{m}}{\partial z}+\frac{\partial \psi_{l-1}^{m}}{\partial z}\right)+\left[\left(\frac{\partial \psi_{l+1}^{m-1}}{\partial x}-\frac{\partial \psi_{l-1}^{m-1}}{\partial x}\right) b_{l}^{m}+\left(\frac{\partial \psi_{l+1}^{m+1}}{\partial x}+\frac{\partial \psi_{l-1}^{m+1}}{\partial x}\right) c_{l}^{m}\right] \\
+\left[\left(\frac{\partial \varphi_{l+1}^{m-1}}{\partial y}-\frac{\partial \varphi_{l-1}^{m-1}}{\partial y}\right) b_{l}^{m}+\left(\frac{\partial \varphi_{l+1}^{m+1}}{\partial y}-\frac{\partial \varphi_{l-1}^{m+1}}{\partial y}\right) c_{l}^{m}\right]+2 \sum_{t} \psi_{l}^{m}=2 \sum_{s, l} \psi_{l}^{m}+2 s_{l}^{m} m \text { even } \\
2 i a_{l}^{m}\left(\frac{\partial \varphi_{l+1}^{m}}{\partial z}+\frac{\partial \varphi_{l-1}^{m}}{\partial z}\right)+i\left[\left(\frac{\partial \varphi_{l+1}^{m+1}}{\partial x}-\frac{\partial \varphi_{l-1}^{m+1}}{\partial x}\right) c_{l}^{m}+\left(\frac{\partial \varphi_{l+1}^{m-1}}{\partial x}-\frac{\partial \varphi_{l-1}^{m-1}}{\partial x}\right) b_{l}^{m}\right] \\
\frac{1}{i}\left[\left(\frac{\partial \psi_{l+1}^{m+1}}{\partial y}-\frac{\partial \psi_{l-1}^{m+1}}{\partial y}\right) c_{l}^{m}+\left(\frac{\partial \psi_{l+1}^{m-1}}{\partial y}-\frac{\partial \psi_{l-1}^{m-1}}{\partial y}\right) b_{l}^{m}\right]+2 i \Sigma_{t} \varphi_{l}^{m}=2 \Sigma_{s, l} \varphi_{l}^{m}+2 i s_{l}^{m} m \text { odd }
\end{array}\right.
$$

The coefficients $s_{l}^{m}$ and $\varsigma_{l}^{m}$ stem from the expansion of the source onto spherical harmonics: $S_{l}^{m}=s_{l}^{m}+i \varsigma_{l}^{m}$ and $S(\vec{r}, \vec{\Omega})=\sum_{l=0}^{l=+n} \sum_{m=-1}^{m=+l} S_{l}^{m}(\vec{r}) Y_{l}^{m}(\vec{\Omega})$. The following coefficients are recalled:

$$
\begin{gathered}
a_{l}^{m}=\sqrt{\frac{(l+m+1)(l+1-m)}{(2 l+1)(2 l+3)}} \quad b_{l}^{m}=\sqrt{\frac{(l-m)(l-m-1)}{(2 l+1)(2 l+3)}} \\
c_{l}^{m}=\sqrt{\frac{(l+m+1)(l+m+2)}{(2 l+1)(2 l+3)}}
\end{gathered}
$$

For cylindrical or spherical geometries, the gradient operator should be modified. The coupling of the spatial derivatives of the flux moments implies that the spherical harmonics method is costly in terms of calculations.

### 9.6.2 $\quad \mathrm{P}_{1}$ Approximation

Restricting the flux expansion to order 1, it is expressed with four terms:

$$
\Phi(\vec{r}, \vec{\Omega})=\Phi_{0}^{0}(\vec{r}) Y_{0}^{0}(\vec{\Omega})+\Phi_{1}^{-1}(\vec{r}) Y_{1}^{-1}(\vec{\Omega})+\Phi_{1}^{0}(\vec{r}) Y_{1}^{0}(\vec{\Omega})+\Phi_{1}^{1}(\vec{r}) Y_{1}^{1}(\vec{\Omega})
$$

Instead of identifying the coefficients of the spherical harmonics in the transport equation as previously, this equation is projected on a particular harmonic by multiplying by the conjugate $\overline{Y_{0}^{0}}$, then successively by $\overline{Y_{1}^{-1}}, \overline{Y_{1}^{0}}$, and $\overline{Y_{1}^{1}}$ to reach the moments of the equation after integration over $\vec{\Omega}$. The streaming terms contain the integration of three spherical harmonic terms. The latter can be calculated using the following properties of spherical harmonics:

$$
\begin{gathered}
\int_{\vec{\Omega}} Y_{l_{1}}^{n_{1}}(\vec{\Omega}) Y_{l_{2}}^{n_{2}}(\vec{\Omega}) Y_{l_{3}}^{n_{3}}(\vec{\Omega}) d \vec{\Omega}=0 \quad \text { when } \begin{array}{c}
m_{1}+m_{2}+m_{3} \neq 0 \\
\text { or if } \\
l_{1}+l_{2}+l_{3} \text { odd }
\end{array} \\
\int_{\vec{\Omega}} Y_{0}^{0} Y_{l_{2}}^{n_{2}}(\vec{\Omega}) Y_{l_{3}}^{n_{3}}(\vec{\Omega}) d \vec{\Omega}=\frac{1}{\sqrt{4 \pi}} \int_{\vec{\Omega}} Y_{l_{2}}^{n_{2}}(\vec{\Omega}) Y_{l_{3}}^{n_{3}}(\vec{\Omega}) d \vec{\Omega} \text { since } Y_{0}^{0}=\frac{1}{\sqrt{4 \pi}}
\end{gathered}
$$

The moments projected on the basis formed by the four terms of the spherical harmonics expansion at order $P_{1}$ are obtained through these integrals using Eq. (9.28) and the orthogonality relations:

$$
\left\{\begin{array}{l}
\int_{4 \pi} Y_{1}^{1}(\vec{\Omega}) Y_{1}^{m}(\vec{\Omega}) d \vec{\Omega}=0 \quad \text { for } m \neq-1 \quad \int_{4 \pi} Y_{0}^{0} Y_{0}^{0} d \vec{\Omega}=1 \\
\int_{4 \pi} Y_{1}^{1}(\vec{\Omega}) Y_{1}^{-1}(\vec{\Omega}) d \vec{\Omega}=-\int_{4 \pi} Y_{1}^{1}(\vec{\Omega}) \bar{Y}_{1}^{-1}(\vec{\Omega}) d \vec{\Omega}=-1
\end{array}\right.
$$

$\begin{cases}\text { projection on } Y_{0}^{0} & -\sqrt{\frac{1}{6}} \frac{\partial \Phi_{1}^{1}}{\partial x}-i \sqrt{\frac{1}{6}} \frac{\partial \Phi_{1}^{1}}{\partial y}+\sqrt{\frac{1}{6}} \frac{\partial \Phi_{1}^{-1}}{\partial x}-i \sqrt{\frac{1}{6}} \frac{\partial \Phi_{1}^{-1}}{\partial y}+\sqrt{\frac{1}{3}} \frac{\partial \Phi_{1}^{0}}{\partial z}+\sum_{t} \Phi_{0}^{0}=\sum_{s, 0} \Phi_{0}^{0}+S_{0}^{0} \\ \text { projection on } Y_{1}^{-1} & \sqrt{\frac{1}{6}} \frac{\partial \Phi_{0}^{0}}{\partial x}+i \sqrt{\frac{1}{6}} \frac{\partial \Phi_{0}^{0}}{\partial y}+\sum_{t} \Phi_{1}^{-1}=\sum_{s, 1} \Phi_{1}^{-1}+S_{1}^{-1} \\ \text { projection on } Y_{1}^{0} & \sqrt{\frac{1}{3}} \frac{\partial \Phi_{0}^{0}}{\partial z}+\sum_{t} \Phi_{1}^{0}=\sum_{s, 1} \Phi_{0}^{0}+S_{1}^{0} \\ \text { projection on } Y_{1}^{1} & -\sqrt{\frac{1}{6}} \frac{\partial \Phi_{0}^{0}}{\partial x}+i \sqrt{\frac{1}{6}} \frac{\partial \Phi_{0}^{0}}{\partial y}+\sum_{t} \Phi_{1}^{1}=\sum_{s, 1} \Phi_{1}^{1}+S_{1}^{1}\end{cases}$
These equations deal with the real moments $\left(\Phi_{0}^{0}, \Phi_{1}^{0}\right)$ or complex moments $\left(\Phi_{1}^{-1}\right.$, $\Phi_{1}^{1}$ ) of the flux. The integrated flux and current, which are usual quantities used in neutron physics, are obtained by writing:

Integrated flux: $\quad \Phi(\vec{r})=\int_{\Omega} \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}=\sqrt{4 \pi} \Phi_{0}^{0}$
Integrated current: $\vec{J}(\vec{r})=\left(\begin{array}{c}J_{x}=\int_{\vec{\Omega}} \sin \theta \cos \varphi \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}=\sqrt{\frac{2 \pi}{3}}\left(\Phi_{1}^{-1}-\Phi_{1}^{1}\right) \\ J_{y}=\int_{\vec{\Omega}} \sin \theta \cos \varphi \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}=-i \sqrt{\frac{2 \pi}{3}}\left(\Phi_{1}^{-1}+\Phi_{1}^{1}\right) \\ J_{z}=\int_{\vec{\Omega}} \cos \theta \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}=\sqrt{\frac{4 \pi}{3}} \Phi_{1}^{0}\end{array}\right)$
By adding and subtracting the projections on $Y_{1}^{-1}$ and $Y_{1}^{1}, \Phi_{1}^{-1}+\Phi_{1}^{1}$ and $\Phi_{1}^{-1}$ $-\Phi_{1}^{1}$ can be introduced, and therefore, by injecting the integrated flux and current, we obtain:

$$
\left\{\begin{array}{l}
\underbrace{\left(\frac{\partial J_{x}}{\partial x}+\frac{\partial J_{y}}{\partial x}+\frac{\partial J_{z}}{\partial z}\right)}_{d i v \vec{J}}+\sum_{t} \Phi=\sum_{s, 0} \Phi+\sqrt{4 \pi} S_{0}^{0} \\
\frac{1}{3} \frac{\partial \Phi}{\partial x}+\Sigma_{t} J_{x}=\Sigma_{s, 1} J_{x}+\sqrt{\frac{2 \pi}{3}}\left(S_{1}^{-1}-S_{1}^{1}\right) \\
\frac{1}{3} \frac{\partial \Phi}{\partial z}+\Sigma_{t} J_{z}=\Sigma_{s, 1} J_{z}+\sqrt{\frac{4 \pi}{3}} S_{1}^{0} \\
\frac{1}{3} \frac{\partial \Phi}{\partial y}+\Sigma_{t} J_{y}=\Sigma_{s, 1} J_{y}+\sqrt{\frac{2 \pi}{3}}\left(S_{1}^{-1}+S_{1}^{1}\right)
\end{array}\right.
$$

These are the usual diffusion equations by using the diffusion coefficient $D \equiv 1 /\left(3\left(\sum_{t}-\sum_{s, 1}\right)\right)$ for the case of a non-isotropic source. It can be pointed out that
the streaming terms could have been written using the spherical harmonics terms $Y_{0}^{2}$, $Y_{2}^{2}, Y_{2}^{0}, Y_{0}^{-2}$ and $Y_{2}^{-2}$ if recurrence relations for spherical harmonics were employed as was the case for the general derivation of the method discussed in the previous paragraph. Once more, just like for the approximation by Legendre polynomials where that paradox was discussed, the transport equation can be approximated by the expansion of a function on $\sum_{l=0}^{2} \sum_{m=-l}^{m=+l} Y_{l}^{m}$ thanks to the streaming term. The number 2 in the previous formula is important as the choice of keeping only the moments of order 1 implies that the choice is arbitrary but logical (i.e. keeping the "first" four moments among the nine moments of the equation). Consequently, the solution obtained does not satisfy the initial equation strictly in each angular direction. It should be noted that at order $n$, the number of moments that satisfy the initial problem is $2 n+1$, while $2 n+3$ do not, given that the total number of moments is $\sum_{l=0}^{2}(2 l+1)=(n+1)^{2}$. The ratio of the non-satisfactory to total moments converges towards 0 as a $2 / n$ series, thereby explaining why the method converges ad infinitum. This progression also explains why the method is quickly very prohibitive in terms of calculation time as the order increases.

### 9.7 Milne Problem

(Busbridge 1960).
A particular interface problem has been of interest to the scientific community at large given that it could be solved analytically: the Milne problem (Picture 9.1). ${ }^{21}$ The latter consists of an interface between a medium and vacuum. For the sake of simplicity, the problem will be considered for mono-kinetic cases only. Any neutron that crosses the medium to vacuum can come back in the negative halfspace (the origin of the abscissa is placed at the interface as in Fig. 9.8) that contains the medium. This condition is expressed as:

$$
\Phi(x, \mu)=0 \quad \text { for } \quad\left\{\begin{array}{l}
x>0 \\
-1 \leq \mu \leq 0
\end{array}\right.
$$

This non-linear problem has been studied in astrophysics to understand the anisotropic nature of radiation that is emitted in the space vacuum. However, a

[^199]

Picture 9.1 Edward Arthur Milne (1896-1950) (Public domain)


Fig. 9.8 Milne problem: neutrons leak into vacuum
linear approximation, called the grey model, may be derived and is easier to solve. The extension for an atmosphere of finite optical thickness is possible (Nonlinear integral equations 1964, p. 345). Vacuum can be assimilated as a black body for which the scattering cross section is zero and the total cross section tends towards infinity. With these assumptions for a purely absorbing medium with uniform internal source, the $\varphi_{l}$ matrix is written as:


The calculation of the first few determinants leads to:

$$
\left\{\begin{aligned}
\operatorname{det} A(0, \lambda) & =\lambda=P_{1}(\lambda) \\
\operatorname{det} A(1, \lambda) & =\left(\begin{array}{cc}
\lambda & -1 \\
-1 & 3 \lambda
\end{array}\right)=3 \lambda^{2}-1=2 P_{2}(\lambda) \\
\operatorname{det} A(2, \lambda) & =\left(\begin{array}{ccc}
\lambda & -1 & 0 \\
-1 & 3 \lambda & -2 \\
0 & -2 & 5 \lambda
\end{array}\right)=5 \lambda\left(3 \lambda^{2}-1\right)-4 \lambda=15 \lambda^{3}-5 \lambda=6 P_{3}(\lambda) \\
\operatorname{det} A(3, \lambda) & =\left(\begin{array}{cccc}
\lambda & -1 & 0 & 0 \\
-1 & 3 \lambda & -2 & 0 \\
0 & -2 & 5 \lambda & -3 \\
0 & 0 & -4 & 7 \lambda
\end{array}\right)=7 \lambda \operatorname{det} A(2, \lambda)-3^{2} \operatorname{det} A(2, \lambda)=24 P_{4}(\lambda)
\end{aligned}\right.
$$

and, more generally, by expanding the determinant along the last line to use the tri-diagonal property of the matrix:

$$
\operatorname{det} A(n, \lambda)=(2 n+1) \lambda \operatorname{det} A(n-1, \lambda)-n^{2} \operatorname{det} A(n-2, \lambda)
$$

From the formulae of the first terms, the general form can be induced as:

$$
\operatorname{det} A(n, \lambda)=(n+1)!P_{n+1}(\lambda)
$$

which can be easily proved by recurrence as:
$\operatorname{det} A(n, \lambda)=(2 n+1) \lambda \operatorname{det} A(n-1, \lambda)-n^{2} \operatorname{det} A(n-2, \lambda)=(2 n+1) \lambda n!P_{n}(\lambda)-n^{2}$ $(n-1)!P_{n-1}(\lambda)$

Using the recurrence relation for Legendre polynomials:

$$
\lambda P_{n}(\lambda)=\frac{n+1}{(2 n+1)} P_{n+1}(\lambda)+\frac{n}{(2 n+1)} P_{n-1}(\lambda)
$$

the following equation is reached:

$$
\begin{aligned}
\operatorname{det} A(n, \lambda)= & (2 n+1) n!\left[\frac{n+1}{(2 n+1)} P_{n+1}(\lambda)+\frac{n}{(2 n+1)} P_{n-1}(\lambda)\right] \\
& -n^{2}(n-1)!P_{n-1}(\lambda) \\
= & (n+1)!P_{n-1}(\lambda)
\end{aligned}
$$

Thus, to conclude, $\lambda_{k}$ are the roots of the Legendre polynomial of order $n+1$ (also known as Gauss points). The reconstructed flux solution (purely scattering medium, source ad infinitum) is given in Fig. 9.9. It can be noted that for incoming angles ( $-1 \leq \mu \leq 0$ ), the solution "oscillates" about 0 while the exact solution is strictly zero, thereby showing the difficulty of calculating interfaces with the $P_{n}$ method.


Fig. 9.9 Milne problem: angular flux at the interface with vacuum, in the case of purely scattering medium with source ad infinitum

## $9.8 \quad D P_{n}$ Method

In the case of an interface, the double $P_{n}$ or double range $P_{n}$ method from Jacques Yvon ${ }^{22,23}$ is more precise than the usual $P_{n}$ method by construction since it expands the angular flux in terms of incoming and outgoing angles (Clark and Hansen 1964,

[^200]p. 196). The flux is then expanded with two different expressions depending on the sign of $\mu$ (Advances Nuclear Science and Technology, vol. 5, p. 333, 1969; Stacey 2001, p. 341):
$$
\Phi(x, \pm \mu)=\sum_{l=0}^{l=n} \frac{(2 l+1)}{2} \Phi_{l}^{ \pm}(x) P_{l}(2 \mu-1)
$$
with: $\Phi_{l}^{ \pm}(x)=2 \int_{0}^{+1} \Phi(x, \pm \mu) P_{l}(2 \mu-1) d \mu$. The flux moment can rewritten as:
$$
\Phi_{l}(x)=\int_{-1}^{0} \Phi(x, \mu) P_{l}(\mu) d \mu+\int_{0}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu=(-1)^{l} \int_{0}^{+1} \Phi(x,-\mu) P_{l}(\mu) d \mu+
$$ $\int_{0}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu$
where $\mu \geq 0$. By injecting these expansions into the integro-differential form of the mono-energy transport equation and by expressing the streaming term $\mu \partial \Phi(x, \pm \mu) \partial x$ as $(1 / 2(2 \mu-1)+1 / 2) \partial \Phi(x, \pm \mu) \partial x$, the following equation is reached:
commissioner of atomic energy from 1970 to 1975, thereby succeeding to Francis Perrin. His portrait is found in (Reuss 2007, p. 58). The CEA has published his complete (significant) works, which cover more than just neutron physics (Yvon 1985).

\[

$$
\begin{aligned}
& \pm\left(\frac{1}{2}(2 \mu-1)+\frac{1}{2}\right) \frac{\partial \Phi(x, \pm \mu)}{\partial x}+\Sigma_{t} \Phi(x, \pm \mu) \\
& =\sum_{l=0}^{\infty}(-1) \frac{l(2 l+1)}{2} \Sigma_{s, l} P_{l}(\mu)\left[(-1)^{l} \int_{0}^{+1} \Phi(x,-\mu) P_{l}(\mu) d \mu+\int_{0}^{+1} \Phi(x, \mu) P_{l}(\mu) d \mu\right] \\
+ & S(x, \pm \mu)
\end{aligned}
$$
\]

This equation with a relatively artificial streaming term is useful for separating the latter into two terms which are added and where the coefficients for the flux derivative, i.e. $(2 \mu-1) / 2$ and $1 / 2$, are always positive, even for $\mu \leq 0$. Using these definitions, the equation is expressed as:

$$
\begin{aligned}
& \pm \frac{1}{2}(2 \mu-1) \sum_{p=0}^{\infty} \frac{(2 p+1)}{2} P_{p}(2 \mu-1) \frac{\partial \Phi_{p}^{ \pm}(x)}{\partial x} \pm \frac{1}{2} \sum_{p=0}^{\infty} \frac{(2 p+1)}{2} P_{p}(2 \mu-1) \frac{\partial \Phi_{p}^{ \pm}(x)}{\partial x} \\
& \quad+\Sigma_{t} \sum_{p=0}^{\infty} \frac{(2 p+1)}{2} P_{p}(2 \mu-1) \partial \Phi_{p}^{ \pm}(x) \\
& =\sum_{p=0}^{\infty}(-1)^{l} \frac{(2 l+1)}{2} \Sigma_{s, l} P_{l}(\mu)\left[\begin{array}{l}
\left.(-1)^{l} \int_{0}^{+1}\left[\sum_{p^{\prime}=0}^{\infty} \frac{\left(2 p^{\prime}+1\right)}{2} P_{p^{\prime}}(2 \mu+1) \Phi_{p^{\prime}}^{ \pm}(x)\right] P_{l}(\mu) d \mu\right] \\
+\int_{0}^{+1}\left[\sum_{p^{\prime}=0}^{\infty} \frac{\left(2 p^{\prime}+1\right)}{2} P_{p^{\prime}}(2 \mu-1) \Phi_{p^{\prime}}^{ \pm}(x)\right] P_{l}(\mu) d \mu
\end{array}\right] \\
& \quad+S(x, \pm \mu)
\end{aligned}
$$

As for the $P_{n}$ method, the recurrence formula to simplify the leakage term is:

$$
(2 p+1)(2 \mu-1) P_{p}(2 \mu-1)=(p+1) P_{p+1}(2 \mu-1) p P_{p-1}(2 \mu-1) \quad \text { for } n>0
$$

The notations can be sensibly simplified as follows:

$$
\begin{aligned}
& \alpha_{l, p}=2^{l}(2 p+1) \int_{0}^{+1} P_{l}(\mu) P_{p+1}(2 \mu-1) d \mu \\
& =\frac{4 l}{2 l+1} \frac{2 p+1}{p} \alpha_{l-1, p-1}+\frac{l+1}{2 l+1} \frac{2 p+1}{p} \alpha_{l+1, p-1}-\frac{2 p+1}{p} \alpha_{l, p-1}-\frac{(p+1)(2 p+1)}{(2 p-3) p} \alpha_{l, p-2}
\end{aligned}
$$

with the following terms to start the recurrence:

$$
\alpha_{0,0}=1, \alpha_{1,0}=1, \alpha_{2,0}=0, \alpha_{3,0}=-1, \alpha_{5,0}=2, \alpha_{7,0}=-5, \alpha_{l, 0}=\frac{4(2-l)}{l+1} \alpha_{l-2,0}
$$

$$
\begin{gathered}
\alpha_{l, 1}=\frac{12 l}{2 l+1} \alpha_{l-2,0}-3 \alpha_{l, 0}+\frac{3(l+1)}{2 l+1} \alpha_{l+1,0} \\
\pm \frac{1}{2} \sum_{p=0}^{\infty}(p+1) P_{p+1}(2 \mu-1) \frac{\partial \Phi_{p}^{ \pm}(x)}{\partial x} \pm \sum_{p=0}^{\infty} p P_{p-1}(2 \mu-1) \frac{\partial \Phi_{p}^{ \pm}(x)}{\partial x} \pm \frac{1}{2} \sum_{p=0}^{\infty}(p+1) P_{p}(2 \mu-1) \frac{\partial \Phi_{p}^{ \pm}(x)}{\partial x} \\
+\sum_{l} \sum_{p=0}^{\infty}(2 p+1) P_{p}(2 \mu-1) \Phi_{p}^{ \pm}(x)= \\
\frac{1}{2} \sum_{p=0}^{\infty} \frac{(-1)^{l}}{2^{l}}(2 l+1) \Sigma_{s, l} P_{l}(\mu)\left(\sum_{p^{\prime}} \alpha_{l, p^{\prime}} \Phi_{p^{\prime}}^{ \pm}(x)\right)+\frac{1}{2} \sum_{p=0}^{\infty} \frac{1}{2^{l}}(2 l+1) \Sigma_{s, l} P_{l}(\mu)\left(\sum_{p^{\prime}} \alpha_{l, p^{\prime}} \Phi_{p^{\prime}}^{ \pm}(x)\right)+S(x, \pm \mu)
\end{gathered}
$$

The same process as for the $P_{n}$ method is thereby reached and will not be further developed:

- The previous equation is projected on a Legendre polynomial basis by multiplying by $P_{p}(2 \mu-1)$,
- Then after integration on $[0,+1]$ and using the orthogonality relation:

$$
\int_{0}^{+1} P_{l}(2 \mu-1) P_{m}(2 \mu-1) d \mu \frac{\delta_{l, m}}{2 l+1}
$$

### 9.9 Semi-infinite Plane: Albedo Problem

### 9.9.1 Fundamentals of Discrete Eigenfunctions

Since the initial works of K. Case, G. Placzek and Hoffman (Case et al. 1953), several authors have thoroughly studied the case of a medium, which may be multiplying, in an infinite half-space. Semi-analytical solutions are possible for the mono-energy problem and are useful to validate approximated numerical methods. The $1 D$ transport equation with an isotropic fission source is written as:

$$
\left\{\begin{array}{l}
S(x, \vec{\Omega})=\frac{v \Sigma_{f}(x)}{4 \pi} \Phi(x) \quad \text { i.e. } \quad S(x)=\frac{v \Sigma_{f}(x)}{2} \Phi(x, \mu) \\
\mu \frac{\partial \Phi(x, \mu)}{\partial x}+\Sigma_{t}(x) \Phi(x, \mu)=\int_{-1}^{+1}\left[\Sigma_{S}\left(x, \mu^{\prime} \rightarrow \mu\right)+\frac{v \sum_{f}(x)}{2}\right] \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}
\end{array}\right.
$$

Assuming that scattering is isotropic $\left(\Sigma_{S}\left(x, \mu^{\prime} \rightarrow \mu\right)=\Sigma_{s, 0}(x) / 2\right)$ and that the cross sections are constant, therefore, the following equation is obtained:

$$
\mu \frac{1}{\Sigma_{t}} \frac{\partial \Phi(x, \mu)}{\partial x}+\Phi(x, \mu)=\frac{c}{2} \int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}
$$

where $c \equiv\left(v \sum_{f}+\sum_{s, 0}+2 \sum_{n, 2 n}+3 \sum_{n, 3 n}+\ldots\right) / \sum_{t}$ is the average number of secondary neutrons emitted per collision (Stamm'ler and Abbate 1983, p. 16). The following change in variable $\mathrm{x}=\sum_{t} x$ is applied by converting distances into the number of mean free paths, thus leading to the canonical equation:

$$
\mu \frac{\partial \Phi(\mathrm{x}, \mu)}{\partial \mathrm{x}}+\Phi(\mathrm{x}, \mu)=\frac{c}{2} \int_{-1}^{+1} \Phi\left(\mathrm{x}, \mu^{\prime}\right) d \mu^{\prime}
$$

The "classical" approach derived by K. M. Case (Case and Zweifel 1967; Duderstadt and Martin 1979) assumes that the flux may be factorized in angle and space: $\Phi(\mathrm{x}, \mu) \equiv \varphi(\mathrm{x}) \psi(\mu)$. When injected in the transport equation, the resulting equation is equivalent to a usual separation of functions which depend either on space or the angle, and are hence constant ${ }^{24}$ :

$$
\frac{1}{\varphi(\mathrm{x})} \frac{\partial \varphi(\mathrm{x})}{\partial \mathrm{x}}=-\frac{1}{\mu}+\frac{c}{2 \mu \mu(\mu)} \int_{-1}^{+1} \psi\left(\mu^{\prime}\right) d \mu^{\prime}=-\frac{1}{v}
$$

The constant was arbitrarily chosen in the form $1 / v$ so that $v$ has the same "dimensions", at least from a mathematical viewpoint, as $\mu$ (physically $\mu$ is a cosine and thus, dimensionless). The choice for a negative constant implies that the spatial flux $\varphi(\mathrm{x})$ is decreasing in the half-plane. The latter is thus more physical, yet the choice could have been to choose a positive value for an increasing flux depending on the case. The previous expression is integrated and the following equations are reached:

$$
\left\{\begin{array}{l}
\varphi(\mathrm{x})=e^{-\frac{\mathrm{x}}{v}} \\
\left(1-\frac{\mu}{v}\right) \psi_{v}(\mu) \frac{c}{2} \int_{-1}^{+1} \psi_{v}\left(\mu^{\prime}\right) d \mu^{\prime}
\end{array}\right.
$$

The angular part of the flux is indexed by $v$ and is sometimes called the continuous eigenfunction, normalized to unity as:

$$
\int_{-1}^{+1} \psi_{v}(\mu) d \mu=1
$$

[^201]Therefore, $\psi_{v}(\mu) \frac{c v}{2(v-\mu)}$. However, it must be noted that if $\mu=v$, which is physically possible, this equation is senseless! Applying the normalization to the flux thus computed, we obtain the dispersion equation which was discussed in the previous chapter:

$$
\frac{c}{2} \nu \ln \left(\frac{\nu+1}{\nu-1}\right)=1
$$

Considering the solution to that equation, it is known that if $c<1$, two real eigenvalues $+v_{0}$ and $-v_{0}$ exist and are the roots of the previous equation. For numerical situations where $+v_{0}>1$, there is no risk that $\mu=+v_{0}$ or $\mu=-v_{0}$ and hence, two discrete eigenfunctions are obtained:

$$
\left\{\begin{array}{l}
\Phi_{+v_{0}}(\mathrm{x}, \mu)=\frac{v_{0} c}{2\left(v_{0}-\mu\right)} e^{+\frac{\mathrm{x}}{v_{0}}} \\
\Phi_{-v_{0}}(\mathrm{x}, \mu)=-\frac{c v_{0}}{2\left(-v_{0}-\mu\right)} e^{-\frac{\mathrm{x}}{v_{0}}}=\frac{c v_{0}}{2\left(v_{0}-\mu\right)} e^{-\frac{\mathrm{x}}{v_{0}}}
\end{array}\right.
$$

If $c=1$, the eigenvalues $\pm v_{0}$ tend towards $\pm \infty$ (since $B=\sum_{t} / v$ tends towards 0 in the dispersion equation). From the transport equation, it can be easily proved that two linearly-independent eigenfunctions are thus:

$$
\left\{\begin{array}{l}
\Phi_{+v_{0} \rightarrow \infty}(\mathrm{x}, \mu)=\frac{1}{2} \\
\Phi_{+v_{0} \rightarrow \infty}(\mathrm{x}, \mu)=\frac{1}{2}(\mathrm{x}, \mu)
\end{array}\right.
$$

The situation where $v \in[-1,1]$ is more delicate given that $v-\mu$ may cancel out at the denominator (Duderstadt and Martin 1979; Glasstone and Edlund 1972, p. 396). Using the notion of Cauchy integral [notion of the principal value $V_{p}$ (Harper 1976, p. 111; Kanwal 1971, p. 173)], it can be shown that the spectrum of eigenfunctions ${ }^{25}$ is continuous:

$$
\begin{aligned}
\psi_{v}(\mu) & =\frac{v c}{2} V_{P}\left[\frac{1}{(v-\mu)}\right]+A(v) \delta(v-\mu) \\
\text { with: } \int_{-1}^{+1} V_{P}\left[\frac{1}{(\nu-\mu)}\right] d \mu & =\lim _{\varepsilon \rightarrow 0}\left(\int_{-1}^{\nu-\varepsilon} \frac{1}{(\nu-\mu)} d \mu+\int_{\nu+\varepsilon}^{+1} \frac{1}{(\nu-\mu)} d \mu\right) \\
& =\lim _{\varepsilon \rightarrow 0}\left[\ln \left(\frac{\nu+1}{\nu-1}\right)-\ln \varepsilon+\ln \varepsilon\right]
\end{aligned}
$$

[^202]Fig. 9.10 Infinite halfspace with incident monodirectional source


The function $A(v)$ is obtained by the normalization condition:

$$
A(\nu)=1-\frac{c \nu}{2} \int_{-1}^{+1} \frac{1}{\nu-\mu} d \mu=1-\frac{c \nu}{2} \ln \left(\frac{\nu+1}{\nu-1}\right)=1-c \nu \operatorname{Arg} \tanh (\nu)
$$

The roots of the function $A(v)$ correspond to the dispersion equation studied by K. M. Case in an approximated approach as established in Chap. 8. For a source of mono-directional neutrons in direction $\mu_{0}=\cos \theta_{0}$ which radiates on an infinite slab (Fig. 9.10), i.e. with boundary conditions $\Phi(0, \mu)=\delta\left(\mu-\mu_{0}\right)$ and the flux that tends towards zero at infinity: $\lim _{x \rightarrow+\infty} \Phi(\mathrm{x}, \mu)=0$, the solution of the transport equation in the slab is expressed as:

$$
\begin{cases}\Phi\left(\mathrm{x}, \mu, \mu_{0}\right)=\delta\left(\mu-\mu_{0}\right) e^{-\frac{\mathrm{x}}{\mu_{0}}}+\frac{c}{2 \mu} \int_{0}^{\mathrm{x}} d \mathrm{x}^{\prime} e^{-\frac{\left(\mathrm{x}-\mathrm{x}^{\prime}\right)}{\mu}} \Phi\left(\mathrm{x}^{\prime}, \mu_{0}\right) & \text { for } \mu \geq 0 \\ \Phi\left(\mathrm{x},-\mu, \mu_{0}\right)=\frac{c}{2 \mu} \int_{x}^{+\infty} d \mathrm{x}^{\prime} e^{-\frac{\left(\mathrm{x}^{\prime}-\mathrm{x}\right)}{\mu}} \Phi\left(\mathrm{x}^{\prime}, \mu_{0}\right) & \text { for }-\mu \leq 0\end{cases}
$$

with $\Phi\left(\mathrm{x} ; \mu_{0}\right)=\int_{-1}^{+1} d \mu^{\prime} \Phi\left(\mathrm{x}, \mu^{\prime} ; \mu_{0}\right)$. Ganapol et al. published a well-documented paper on the subject matter. ${ }^{26}$ Here, the same notations as Ganapol et al. will be

[^203]employed with the use of $\mu_{0}$ in the angularly-integrated flux for clarity. Integrating on the interval $[0,1]$ for incoming directions in the slab $(\mu \geq 0)$ leads to:
$$
\Phi\left(\mathrm{x}, \mu_{0}\right)=e^{-\frac{\mathrm{x}}{\mu^{0}}}+\frac{c}{2} \int_{0}^{\mathrm{x}} d \mathrm{x}^{\prime} E_{1}\left(\left|\mathrm{x}-\mathrm{x}^{\prime}\right|\right) \Phi\left(\mathrm{x}^{\prime}, \mu_{0}\right)
$$
and, in terms of the $x$-coordinate which has the same dimensions as a length:
$$
\Phi\left(x, \mu_{0}\right)=e^{-\frac{\Sigma_{x x}}{\mu 0}}+\frac{c}{2} \int_{0}^{\mathrm{x}} d \mathrm{x}^{\prime} E_{1}\left(\Sigma_{t}\left|x-x^{\prime}\right|\right) \Phi\left(x^{\prime}, \mu_{0}\right)
$$
with the exponential integral: $E_{1}(x)=\int_{1}^{\infty} e^{-x t} / t d t$. Differentiating this equation wrt. $x$, the integro-differential equation for $\Phi\left(x ; \mu_{0}\right)$ is reached:
$$
\frac{\partial \Phi\left(\mathrm{x}, \mu_{0}\right)}{\partial \mathrm{x}}+\frac{\Phi\left(\mathrm{x}, \mu_{0}\right)}{\mu_{0}}=\frac{c}{2} \Phi\left(0, \mu_{0}\right) \int_{0}^{1} d \mu^{\prime} \frac{\Phi\left(\mathrm{x}, \mu^{\prime}\right)}{\mu}
$$

A direct analysis of the angular flux expression leads to the reciprocity relation:

$$
\mu \Phi\left(\mathrm{x},-\mu, \mu_{0}\right)=\mu_{0} \Phi\left(\mathrm{x},-\mu_{0}, \mu\right)
$$

Multiplying the previous integro-differential equation by $e^{-x / \mu}$ and integrating the resulting equation over $\mathrm{x} \in[0,+\infty]$, the following reciprocity relation is reached:

$$
\Phi\left(\mathrm{x},-\mu, \mu_{0}\right)=\frac{c}{2} \frac{\mu_{0}}{\mu_{0}+\mu} \Phi\left(\mathrm{x}, \mu_{0}\right) \Phi(0, \mu)
$$

As Ganapol points out, $\Phi(0, \mu)$ is simply the function that Subrahmanyan Chandrasekhar ${ }^{27}$ (1910-1995) employs in his treatise on radiative transfer under

[^204]the notation $H(\mu)^{28}$ (Chandrasekhar 1960, p. 105; Busbridge 1960, p. 13; Shultis and Faw 2000, p. 442). With these notations, the outgoing angular flux is written as:
$$
\Phi\left(\mathrm{x},-\mu, \mu_{0}\right)=\frac{c}{2} \frac{\mu_{0}}{\mu_{0}+\mu} H\left(\mu_{0}\right) H(\mu)
$$

The function $H(\mu)$ satisfies the non-linear integral equation:

$$
\begin{equation*}
\text { Chandrasekhar function: } \quad H(\mu)=1+\frac{c}{2} \mu H(\mu) \int_{0}^{1} \frac{H\left(\mu^{\prime}\right)}{\mu^{\prime}+\mu} d \mu^{\prime} \text { with } c \in[0,1] \tag{9.29}
\end{equation*}
$$

At the slab surface, the outgoing angular flux is equal to:

$$
\Phi\left(0,-\mu, \mu_{0}\right)=\frac{c}{2 \mu} \int_{x}^{+\infty} d \mathrm{x}^{\prime} e^{-\frac{x^{\prime}}{\mu}} \Phi\left(\mathrm{x}^{\prime}, \mu_{0}\right)
$$



Subrahmanyan Chandrasekhar (Public domain)
${ }^{28}$ Chandrasekhar defines a class of functions that are more general $H(\mu)=1+\mu H(\mu) \int_{0}^{1} \frac{\Psi\left(\mu^{\prime}\right)}{\mu^{\prime}+\mu} d \mu^{\prime}$ where $\Psi$ is a characteristic function in the form of a polynomial in $\mu$ such that $\int_{0}^{1} \Psi(\mu) d \mu \leq 1$. A numerical smoothening of $H(\mu)$ in terms of $\mu$ and $\sum_{s} / \sum_{t}$ is discussed in: Ronald C. Brockhoff, J. Kenneth Shultis: A new approach for the neutron albedo, Nuclear Science and Engineering, 155, pp. 1-17 (2007).

### 9.9.2 Ganapol Method by Laplace Transform



Barry Ganapol (1944-) is a renowned transport theory specialist (Courtesy Ganapol)
If $\mu$ is substituted by the complex variable $1 / p$, the above equation is the Laplace transform ${ }^{29}$ of the function $\Phi\left(\mathrm{x}^{\prime} ; \mu_{0}\right)$ :

$$
\Phi\left(0,-\frac{1}{p}, \mu_{0}\right)=\frac{c p}{2} \int_{x}^{+\infty} d \mathrm{x}^{\prime} e^{-p \mathrm{x}^{\prime}} \Phi\left(\mathrm{x}^{\prime}, \mu_{0}\right)
$$

The inverse of this Laplace transform can be obtained by the Bromvitch inversion formula:

$$
\Phi\left(\mathrm{x}, \mu_{0}\right)=\frac{2}{c} \frac{1}{2 \pi i} \int_{\gamma-i \infty}^{\gamma+i \infty} \frac{1}{p} \Phi\left(0,-\frac{1}{p}, \mu_{0}\right) e^{p \mathrm{x}} d p
$$

The analytical angular flux solution in terms of the Chandrasekhar function is given by:

$$
\Phi\left(\mathrm{x},-\frac{1}{p}, \mu_{0}\right)=\frac{c}{2} \frac{p \mu_{0}}{\mu_{0} p+1} H\left(\mu_{0}\right) H\left(\frac{1}{p}\right)
$$

where: $\Phi\left(\mathrm{x}, \mu_{0}\right)=\mu_{0} H\left(\mu_{0}\right) \frac{1}{2 \pi i} \int_{\gamma-i \infty}^{\gamma+i \infty} \frac{1}{\mu_{0} p+1} H\left(\frac{1}{p}\right) e^{p \mathrm{x}} d p$

[^205]The complex integral can be calculated either with the residue theorem or by calculating the inverse Laplace transform numerically. Ganapol extends this approach to the flux $\Phi_{0}(\mu)$ imposed at the surface. The $\Phi(x, \mu)$ flux is the angular Green function:

$$
\Phi(\mathrm{x}, \mu)=\int_{0}^{1} \Phi\left(\mu^{\prime}\right) \Phi\left(\mathrm{x}, \mu, \mu^{\prime}\right) d \mu^{\prime}
$$

Thus, the outgoing flux is: $\Phi(0,-\mu)=\frac{c}{2} H(\mu) \int_{0}^{1} \Phi_{0}\left(\mu^{\prime}\right) \frac{\mu^{\prime}}{\mu+\mu^{\prime}} H\left(\mu^{\prime}\right) d \mu^{\prime}$
Hence, the scalar flux in the half-space is:

$$
\Phi(\mathrm{X})=\mathrm{L}_{\mathrm{X}}^{-1}\left[H\left(\frac{1}{p}\right) \int_{0}^{1} \Phi_{0}\left(\mu^{\prime}\right) \frac{\mu^{\prime}}{1+\mu^{\prime} p} H\left(\mu^{\prime}\right) d \mu^{\prime}\right]
$$

by noting that $\mathrm{L}_{\mathrm{x}}^{-1}(f(p))=\frac{1}{2 \pi i} \int_{\gamma-i \infty}^{\gamma+i \infty} f(p) e^{p \mathrm{x}} d p$ is the inverse Laplace transform.
The Milne problem has been discussed previously for a source at infinity, and located in the right half-space, thereby creating an interface current. It can be solved by this approach assuming that the asymptotic flux at infinity has an exponential form given by the discrete eigenmode presented earlier:

$$
\Phi(\mathrm{x}, \mu)=\Phi_{v}(-\mu) e^{B x}=\Phi_{v}(-\mu) e^{\frac{x}{v_{0}}} \quad \text { when } \quad \mathrm{x} \rightarrow+\infty
$$

where $v_{0}=\Sigma_{t} / B$ is the solution to the Placzek dispersion equation discussed earlier [expressed with the variable $v_{0}$ here for consistence with Case's notations (Duderstadt and Martin 1979)]:

$$
\frac{c}{2} \nu_{0} \ln \left(\frac{\nu_{0}+1}{\nu_{0}-1}\right)=1
$$

This exponential flux, which tends to infinity at infinity, implies that the source placed at infinity must have an infinite intensity to induce a current at the interface (Fig. 9.11).

Duderstadt and Martin (1979) gives an approximation of the extrapolation distance for Milne problem:

$$
d_{0}=0.710446\left(\frac{1}{c}-0.0199 \frac{(1-c)^{3}}{c}+O\left(\frac{(1-c)^{3}}{c}\right)\right)
$$

Fig. 9.11 Infinite halfspace: Milne problem (from Duderstadt and Martin 1979)


This quantity will be used in more advanced techniques for dealing with the physics of neutron reflectors. With the direction of the coordinate system chosen as such, the void boundary condition at the left of the interface is written for incoming directions: $\Phi(\mathrm{x}, v)=0$. The previous problem is obtained with a function that tends towards 0 at infinity by constructing the following function:

$$
\Psi(\mathrm{x}, \mu) \equiv \Phi_{v}(-\mu) e^{\frac{\mathrm{x}}{\mathrm{x}_{0}}}-\Phi(\mathrm{x}, \mu)
$$

that satisfies the same transport equation as $\Phi(\mathrm{x}, \mu)$ :

$$
\mu \frac{\partial \Psi(\mathrm{x}, \mu)}{\partial \mathrm{x}}+\Psi(\mathrm{x}, \mu)=\frac{c}{2} \int_{-1}^{+1} \Psi\left(\mathrm{x}, \mu^{\prime}\right) d \mu^{\prime}
$$

and for which the boundary condition at the interface is: $\Psi\left(0, \mu^{\prime}\right)=\Phi_{v}(-\mu)$. The same calculation procedure as for the calculation of the function $\Psi(\mathrm{x}, \mu)$ may be applied to obtain the outgoing flux:

$$
\Psi(0,-\mu)=\left(\frac{c}{2}\right)^{2} v_{0} H(\mu) \int_{0}^{1} \frac{\mu^{\prime}}{\left(\mu^{\prime}+\mu\right)\left(\mu^{\prime}+v_{0}\right)} H\left(\mu^{\prime}\right) d \mu^{\prime}=\Phi_{v}(\mu)-\frac{c}{2} \frac{v_{0}}{\mu-v_{0}} \frac{H(\mu)}{H\left(v_{0}\right)}
$$

Finally: $\Phi(0,-\mu)=\frac{c}{2} \frac{v_{0}}{\mu-v_{0}} \frac{H(\mu)}{H\left(v_{0}\right)}$
Then, using the same technique described earlier:

$$
\Phi(\mathrm{x}) \frac{v_{0}}{H\left(v_{0}\right)} \mathrm{L}_{\mathrm{x}}^{-1}\left(\frac{H\left(\frac{1}{p}\right)}{v_{0} p-1}\right)
$$

Ganapol generalizes this approach to two adjacent half-spaces with different properties by separating the flux as the uncollided flux and the collided flux. Similarly, for the continuous-lethargy ( $u$, while accounting for the slowing-down
without upscattering) transport equation, the following equation is obtained by starting with the integro-differential equation:

$$
\mu \frac{\partial \Phi(\mathrm{x}, \mu, u)}{\partial \mathrm{x}}+\Phi(\mathrm{x}, \mu, u)=\frac{1}{2} \int_{-1}^{+1} d \mu^{\prime} \int_{0}^{u} d u^{\prime} \underbrace{\frac{2 \Sigma_{s}\left(\mu^{\prime} \rightarrow \mu, u^{\prime} \rightarrow u\right)}{\Sigma_{t}(u)}}_{f\left(u-u^{\prime}\right)} \Phi\left(\mathrm{x}, \mu^{\prime}, u^{\prime}\right)
$$

The coefficient $1 / 2$ is added artificially in front of the integral term to introduce a form of the integro-differential equation which is very similar to the kernel employed for isotropic collision. The interface condition is a mono-energy beam with one incident direction $\mu_{0}$, and with a zero-flux condition at infinity as boundary condition:

$$
\left\{\begin{array}{l}
\Phi(0, \mu, u)=\delta\left(\mu-\mu_{0}\right) \delta(u) \text { for } \mu>0 \\
\lim _{x \rightarrow+\infty} \Phi(\mathrm{x}, \mu, u)=0
\end{array}\right.
$$

A Laplace transform with lethargy $u$ is applied to the transport equation:

$$
\left\{\begin{array}{l}
\mu \frac{\partial \Phi(\mathrm{x}, \mu, p)}{\partial \mathrm{x}}+\Phi(\mathrm{x}, \mu, p)=\frac{\mathrm{F}(p)}{2} \int_{-1}^{+1} d \mu^{\prime} \Phi\left(\mathrm{x}, \mu^{\prime}, p\right) \\
\Phi(\mathrm{x}, \mu, p)=\delta\left(\mu-\mu_{0}\right)
\end{array}\right.
$$

where $\Phi$ and F are the Laplace transforms of $\Phi$ and $f$. This transformation is equivalent to a monoenergy equation to which the previous results obtained earlier may be applied, especially:

$$
\left\{\begin{array}{l}
\Phi(0,-\mu, p)=\frac{\mathrm{F}(p)}{2} \frac{\mu_{0}}{\mu_{0}+\mu} H\left(\mu_{0}, p\right) H(\mu, p) \quad \text { at the surface } \\
\Phi(\mathrm{x}, p)=\frac{1}{\mathrm{~F}(p)} \mathrm{L}_{\mathrm{x}}^{-1}\left[\frac{\Phi\left(\mathrm{x},-\frac{1}{p}, p\right)}{p}\right] \quad \text { in the half-space }
\end{array}\right.
$$

where: $H(\mu, p)=1+\frac{\mathrm{F}(p)}{2} \mu H(\mu, p) \int_{0}^{1} \frac{H(\mu, p)}{\mu^{\prime}+\mu} d \mu^{\prime}$ is the extension of the Chandrasekhar function for the image $\mathrm{F}(p)$. Ganapol expanded the function $H(\mu, p)$ into a series which represents the successive collisions so as to represent the dependence in lethargy:

$$
H(\mu, p)=\sum_{n=0}^{\infty} \mathrm{F}_{n}(p) h_{n}(\mu)
$$

Fig. 9.12 Slowing-down probability in terms of the lethargy step (elastic collision)


Injecting this series into the integro-differential equation on $H(\mu, p)$ leads to the recurrence relations for the coefficients $h_{n}(\mu)$ :

$$
\left\{\begin{array}{l}
h_{0}(\mu)=1 \\
h_{n}(\mu)=\frac{\mu}{2} \sum_{l=0}^{n-1} h_{n-l-1}(\mu) \int_{0}^{1} \frac{h_{l}\left(\mu^{\prime}\right) d \mu^{\prime}}{\mu^{\prime}+\mu}
\end{array}\right.
$$

which results into the following when introduced in the flux expression:

$$
\left\{\begin{array}{l}
\Phi(0,-\mu, p)=\frac{1}{2} \frac{\mu_{0}}{\mu_{0}+\mu} \sum_{n=1}^{\infty} \mathrm{F}_{n}(p) \sum_{l=0}^{n-1} h_{n-l-1}(\mu) h_{l}\left(\mu_{0}\right) \quad \text { at the surface } \\
\Phi(\mathrm{x}, p)=\mu_{0} \sum_{n=1}^{\infty} \mathrm{F}_{n}(p) \sum_{l=0}^{n-1} h_{l}\left(\mu_{0}\right) \mathrm{L}_{\mathrm{x}}^{-1}\left[\frac{h_{n-l}\left(\frac{1}{p}\right)}{\mu_{0} p+1}\right] \quad \text { in the half-space }
\end{array}\right.
$$

This formulation is interesting for calculating a flux series (pseudo-) analytically, if the inverse of the Laplace transform $\mathrm{F}_{n}(p)$ may be computed. The elastic scattering kernel is such an example as discussed in the chapter on slowing-down:

$$
f\left(u-u^{\prime}\right)=c \frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} \Theta\left(u-u^{\prime}\right) \Theta\left(u-u^{\prime}+\varepsilon\right)
$$

where $\Theta$ is the Heaviside step function. ${ }^{30}$
The Laplace transform of this function is written as (Fig. 9.12):

$$
\mathrm{F}(p)=\frac{c}{1-\alpha} \frac{1-e^{-(p+1) \varepsilon}}{p+1}
$$

and the kernel for the number of neutrons reaching lethargy $u$ in exactly $n$ collisions ${ }^{31}$ is written using the binomial coefficients:

[^206]$$
F_{n}(u)=\left(\frac{c}{1-\alpha}\right)^{n} \frac{e^{-u}}{(n-1)!} \sum_{k=1}^{E[u / \varepsilon]}(-1)^{k} C_{n}^{k}(u-k \varepsilon)^{n-1}
$$
where $E[u / \varepsilon]$ is the integer part and $C_{n}^{k}=\frac{n!}{k!(n-k)!}$ is the binomial coefficient (combination of $k$ items among $n$ ). This formula counts the number of times that the lethargy $u$ is reached after exactly $n$ collisions, a collision causing an increase in lethargy by $k \varepsilon$ and a new collision leading to an increase of $(n-k) \varepsilon$. Using these notations:
\[

\left\{$$
\begin{array}{l}
\Phi(0,-\mu, u)=\frac{1}{2} \frac{\mu_{0}}{\mu_{0}+\mu} \sum_{n=1}^{\infty} \mathrm{F}_{n}(u) \sum_{l=0}^{n-1} h_{n-l-1}(\mu) h_{l}\left(\mu_{0}\right) \quad \text { at the surface } \\
\Phi(\mathrm{x}, u)=\delta(u) e^{-\frac{\mathrm{x}}{\mu_{0}}}+\mu_{0} \sum_{n=1}^{\infty} \mathrm{F}_{n}(u) \sum_{l=0}^{n-1} h_{l}\left(\mu_{0}\right) \sum_{l=0}^{n} h_{l}\left(\mu_{0}\right) \mathrm{L}_{\mathrm{x}}^{-1}\left[\frac{h_{n-l}\left(\frac{1}{p}\right)}{\mu_{0} p+1}\right]
\end{array}
$$\right.
\]

The extension to a more realistic boundary condition with a factorizable form in angle and lethargy $\Phi(0, \mu, u)=\varphi(\mu) \phi(u)$, is obtained by composition of the solutions for a given angle and lethargy. This extension is possible assuming that the equation for a discrete boundary condition characterizes the partial Green function in angle and lethargy.

## $9.10 \quad B_{n}$ Method

The $B_{n}$ method consists in expanding the differential scattering cross section on a Legendre polynomial basis without any hypothesis on the flux. The Fourier transform of the latter is (Bekurts and Wirtz 1964, p. 161; Ferziger and Zweifel 1966, p. 182; J. Ernest Wilkins, Robert L. Hellens, Paul F. Zweifel, in Atoms for peace, vol. V, p. 67, 1955):

$$
\varphi(B, \mu)=\int_{-\infty}^{+\infty} e^{-i B x} \Phi(x, \mu) d x
$$

The parameter $B$ in the Fourier transform can take any value (such that even the infinite integral exists and thus, it satisfies at least $\lim _{x \rightarrow \infty} e^{-i B x} \Phi(x, \mu)=0$ ), and its choice may be interpreted physically as demonstrated by Pierre Benoist in 1964. He defined that parameter as the macroscopic leakage from the geometry being considered. For an infinite medium, the flux can be factorized as a macroscopic flux without angular dependence, represented by the buckling $B^{2}$, and a fine periodic flux $\varphi(\vec{r}, E, \vec{\Omega})$, such that $\Phi(\vec{r}, E, \vec{\Omega})=\varphi(\vec{r}, E, \vec{\Omega}) e^{-i, \vec{B}, \vec{r}}$. This approach may
be employed in the calculation of homogenized neutron quantities according to strategies which will be discussed in Chap. 14.

The Fourier transform of the isotropic source term is written as:
Fourier transform of the fission source:

$$
\begin{equation*}
s(B, \mu)=\int_{-\infty}^{+\infty} e^{-i B x} S(x, \mu) d x=\int_{-\infty}^{+\infty} e^{-i B x} S(x, \mu) d x=v \Sigma_{f} \frac{\varphi_{0}(B)}{2} \tag{9.30}
\end{equation*}
$$

Thus, a particular value may be chosen for $B$ and denoted as $B_{m}$ such that it normalizes the Fourier transform of the fission source to one on the lethargy range, i.e.:

$$
\int_{0}^{u_{t h}} v \Sigma_{f} \varphi_{0}\left(B_{m}\right) d u=v \Sigma_{f} \varphi_{0}\left(B_{m}\right) u_{t h}=1
$$

This condition corresponds to a critical medium. Multiplying each term of the $1 D$ transport equation (Eq. 9.14) by $e^{-i B x}$ and integrating between $-\infty$ and $+\infty$, the Fourier transform of the equation thus obtained includes those of the flux $\varphi(B, \mu)$ and the source $s(B, \mu)$ :

Fourier transform of the $1 D$ transport equation :

$$
\begin{equation*}
\left[-\mu i B+\Sigma_{t}\right] \varphi(B, \mu)=\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} \Sigma_{s, l} P_{l}(\mu) \int_{-1}^{+1} P_{l}\left(\mu^{\prime}\right) \varphi\left(B, \mu^{\prime}\right) d \mu^{\prime}+s(B, \mu) \tag{9.31}
\end{equation*}
$$

The Fourier transform of the flux is then expanded in Legendre polynomials:

$$
\varphi_{m}(B, \mu)=\frac{1}{2} \sum_{l=0}^{l=\infty}(2 l+1) \varphi_{l}(B) P_{l}(\mu)
$$

with $\varphi_{l}(B)=\int_{-1}^{+1} \varphi(B, \mu) P_{l}(\mu) d \mu$. Each term of Eq. (9.31) is multiplied by $P_{m}(\mu)$ and then integrated between -1 and +1 , thereby leading to:

$$
\varphi_{m}(B)=\sum_{l=0}^{l=\infty} \frac{2 l+1}{2} \Sigma_{s, l} \varphi_{l}(B) \int_{-1}^{+1} \frac{P_{l}(\mu) P_{m}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu+\int_{-1}^{+1} \frac{s(B, \mu) P_{m}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu
$$

The infinite sum is limited to the expansion order of the scattering cross section. The value of $\varphi_{m}(B)$ is calculated by solving a linear system of equations after the computation of the complex integrals which depend only the total cross section and the source. It should be noted that if $n$ is the expansion order of the scattering cross
section $\left(\Sigma_{s, l>n}=0\right)$, the coefficients $\varphi_{m>n}(B)$ do not depend on the scattering cross section nor on the flux of lower orders but only on the term:

$$
\int_{-1}^{+1} \frac{s(B, \mu) P_{m}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu
$$

Hence, the Fourier transform of the flux is obtained for any order and the inverse transform leads to the neutron flux. This process can be generalized in a multi-group approach by retaining the energy variable and coupling the flux terms through the scattering cross section. The matrix resolution for the groups is then carried out with a triangular slowing-down matrix and a dense thermalization matrix. If the expansion is limited to $B_{1}$, the equations are expressed as:

$$
\left\{\begin{array}{l}
\varphi_{0}(B)=\frac{1}{2} \Sigma_{s, 0} \varphi_{0}(B) \int_{-1}^{+1} \frac{P_{0}(\mu) P_{0}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu+\frac{3}{2} \Sigma_{s, 1} \varphi_{1}(B) \int_{-1}^{+1} \frac{P_{1}(\mu) P_{1}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu+\int_{-1}^{+1} \frac{s(B, \mu) P_{0}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu \\
\varphi_{1}(B)=\frac{1}{2} \Sigma_{s, 0} \varphi_{0}(B) \int_{-1}^{+1} \frac{P_{0}(\mu) P_{1}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu+\frac{3}{2} \Sigma_{s, 1} \varphi_{1}(B) \int_{-1}^{+1} \frac{P_{1}(\mu) P_{1}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu+\int_{-1}^{+1} \frac{s(B, \mu) P_{1}(\mu)}{\left[\Sigma_{t}-\mu i B\right]} d \mu
\end{array}\right.
$$

yet:

$$
\left\{\begin{array}{c}
\int_{-1}^{+1} \frac{s(B, \mu) P_{0}(\mu)}{\left[-\mu i B+\Sigma_{t}\right]} d \mu=\frac{1}{2 B} s_{0}(B) \int_{-1}^{+1} \frac{\left(\frac{\Sigma_{t}}{B}\right)+i \mu}{\left[\mu^{2}+\left(\frac{\Sigma_{t}}{B}\right)^{2}\right]} d \mu=\frac{1}{2} s_{0}(B) \frac{2}{B} A r \tan \left(\frac{B}{\Sigma_{t}}\right)+i \underbrace{\int_{-1}^{+1} \frac{\mu}{\left[\mu^{2}+\left(\frac{\Sigma_{t}}{B}\right)^{2}\right]}}_{-1} d \mu \\
\int_{-1}^{+1} \frac{s(B, \mu) P_{1}(\mu)}{\left[-\mu i B+\Sigma_{t}\right]} d \mu=\frac{1}{2 B} s_{0}(B) \int_{-1}^{+1} \frac{\left(\frac{\Sigma_{t}}{B}\right) \mu+i \mu^{2}}{\left[\mu^{2}+\left(\frac{\Sigma_{t}}{B}\right)^{2}\right]} d \mu=\frac{i}{B} s_{0}(B)\left[1-\frac{\Sigma_{t}}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)\right]
\end{array}\right.
$$

The following equations are finally reached:

$$
\left\{\begin{array}{c}
\varphi_{0}(B)=\frac{1}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)\left[s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B)\right]+\frac{3 i}{B}\left[1-\frac{\Sigma_{t}}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)\right] \Sigma_{s, 1} \varphi_{1}(B) \\
\varphi_{1}(B)=\frac{i}{B}\left[1-\frac{\Sigma_{t}}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)\right]\left[s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B)\right]+\frac{3 \Sigma_{t}}{B^{2}}\left[1-\frac{\Sigma_{t}}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)\right] \Sigma_{s, 1} \varphi_{1}(B)
\end{array}\right.
$$

It can be noted that the combination of the two equations results in:

$$
\varphi_{1}(B)+i \frac{\Sigma_{t}}{B} \varphi_{0}(B)=\frac{i}{B}\left[s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B)\right]
$$

Thus, the Fourier transform of the current is a purely imaginary number (and is simply the first flux moment):

$$
J(B)=\varphi_{1}(B)=\frac{i}{B}\left[s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B)-\Sigma_{t} \varphi_{0}(B)\right]
$$

If the diffusion coefficient is defined as:
Diffusion coefficient: $D(B)=-\frac{i}{B} \frac{\varphi_{1}(B)}{\varphi_{0}(B)}$
the following equation may be written:

$$
\frac{B}{i} \varphi_{1}(B)=D(B) B^{2} \varphi_{0}(B)=s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B)-\Sigma_{t} \varphi_{0}(B)
$$

The material buckling is such that the flux $\varphi_{0}\left(B_{g}\right)$ corresponds to the fundamental mode solution of:

$$
\begin{equation*}
\text { Fundamental mode: } \quad \Delta \varphi_{0}\left(B_{g}\right)+B_{m}^{2} \varphi_{0}\left(B_{g}\right)=0 \tag{9.33}
\end{equation*}
$$

which may be injected in the previous equation for a particular value of $B_{g}$ and hence, the critical diffusion equation is reached:

$$
-D\left(B_{g}\right) \Delta \varphi_{0}\left(B_{g}\right)+\Sigma_{t} \varphi_{0}\left(B_{g}\right)=s_{0}\left(B_{g}\right)+\Sigma_{s, 0} \varphi_{0}\left(B_{g}\right)
$$

Finally, the coefficient $B_{g}^{2}$ has the physical meaning of the geometrical buckling while $D\left(B_{g}\right)$ is the diffusion coefficient associated to the fundamental mode, or even the leakage coefficient. It should be pointed out that since $\varphi_{1}(B)$ is purely imaginary and that $\varphi_{0}(B)$ is a pure real number, $D\left(B_{g}\right)$ is real. The $B_{1}$ method allows calculation of the leakage coefficient corrected of the flux anisotropy effect, but mostly of the buckling in fundamental mode compared to the diffusion coefficient given by the usual $1 /\left(3 \Sigma_{t}\right)$ formula for a homogeneous material. For the $B_{0}$ approximation of isotropic scattering, this correction may be expressed as a factor $\gamma(B, u)$ equal to (Bussac et Reuss 1985):

$$
\left\{\begin{array}{l}
\gamma(B, u)=\frac{1}{3} \frac{\frac{B}{\Sigma_{t}} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)}{1-\frac{B}{\Sigma_{t}} \operatorname{Arc} \tan \left(\frac{B}{\Sigma_{t}}\right)} \approx 1+\frac{1}{15}\left(\frac{B}{\Sigma_{t}}\right)^{2}+O\left(\frac{B}{\Sigma_{t}}\right)^{4} \\
D(u)=\frac{1}{3 \Sigma_{t}(\mu) \gamma(B, u)} \text { in approximation } B_{0} \text { (isotropic scattering) }
\end{array}\right.
$$

In the $B_{1}$ approximation (Stamm'ler and Abbate 1983, p. 365), i.e. for linearlyanisotropic scattering, the leakage coefficient is the solution to an integral equation:

$$
D(u)=\frac{1}{3 \Sigma_{t}(\mu) \gamma(B, u)}\left[1+3 \int_{u^{\prime}} \Sigma_{s_{1}}\left(u^{\prime} \rightarrow u\right) D\left(u^{\prime}\right) \frac{\varphi_{0}\left(u^{\prime}\right)}{\varphi_{0}(u)} d u^{\prime}\right]
$$

The $B_{1}$ approximation allows the leakage calculation with an equivalent precision to the $P_{3}$ approximation. The flux moment $\varphi_{1}$ which is imaginary in the $B_{1}$ approximation can be calculated by writing $\varphi_{1}=i l \varphi_{1} \mid$ so as to express the system $B_{1}$ in real form:

$$
\begin{aligned}
& \left\{\begin{array}{l}
-i B \varphi_{1}(B)+\Sigma_{t} \varphi_{0}(B)=s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B) \\
\gamma(B) \Sigma_{t} \varphi_{1}(B)-i \frac{B}{3} \varphi_{0}(B)=s_{1}(B)+\Sigma_{s, 1} \varphi_{1}(B)
\end{array}\right. \\
& \left\{\begin{array}{l}
B\left|\varphi_{1}(B)\right|+\Sigma_{t} \varphi_{0}(B)=s_{0}(B)+\Sigma_{s, 0} \varphi_{0}(B) \\
\gamma(B) \Sigma_{t}\left|\varphi_{1}(B)\right|-\frac{B}{3} \varphi_{0}(B)=s_{1}(B)+\Sigma_{s, 0}\left|\varphi_{1}(B)\right|
\end{array}\right.
\end{aligned}
$$

If $\Sigma_{s_{1}}=\overline{\mu_{0}} \Sigma_{s_{0}} \delta\left(u-u^{\prime}\right)$, the leakage coefficient may be computed analytically since the integral simplifies into $\overline{\mu_{0}} \Sigma_{s_{0}} D(u)$, i.e.:

$$
D(u)=\frac{1}{3\left(\Sigma_{t}(\mu) \gamma(B, u)-\overline{\mu_{0}} \Sigma_{s_{0}}\right)}
$$

This formula is similar to the one obtained in $B_{0}$ approximation with a transport cross section:

$$
\Sigma_{t r}=\Sigma_{t}(\mu) \gamma(B, u)-\overline{\mu_{0}} \Sigma_{s_{0}}
$$

The Fourier transform method is useful to obtain analytical solutions for simple cases. For instance, for an isotropic plane source, placed at the origin of an infinite medium with constant cross sections, we have $S(x)=\delta(x) / 2$ given that the source emits on both sides of the plane source. Assuming further that scattering is isotropic and thus independent of $\mu_{0}$, the $l D$ transport equation simplifies to:

$$
\mu \frac{\partial \Phi(x, \mu)}{\partial x}+\Sigma_{t} \Phi(x, \mu)=\frac{\Sigma_{s, 0}}{2} \int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}+\frac{\delta(x)}{2} S_{0}
$$

Applying the Fourier transform $\varphi(B, \mu)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i B x} \Phi(x, \mu) d x$ to the previous equation results into:

$$
-i B \mu \varphi(B, \mu)+\Sigma_{t} \varphi(B, \mu)=\frac{\Sigma_{s, 0}}{2} \int_{-1}^{+1} \varphi\left(B, \mu^{\prime}\right) d \mu^{\prime}+\frac{1}{2} S_{0}
$$

This equation is integrated over $\mu$ from -1 to +1 , and thus, the integration of the Fourier transform of the flux can be calculated for the space variable:

Flux Fourier transform: $\quad \varphi(B) \frac{\frac{1}{2} S_{0} \int_{-1}^{+1} \frac{1}{\Sigma_{t}-i B \mu^{\prime}} d \mu^{\prime}}{1-\frac{\Sigma_{s, 0}}{2} \int_{-1}^{+1} \frac{1}{\Sigma_{t}-i B \mu^{\prime}} d \mu^{\prime}}=\frac{\frac{S_{0}}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)}{1-\frac{\Sigma_{s, 0}}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)}$

The flux is then obtained by the inverse Fourier transform of the previous image:

$$
\Phi(x)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{+i B x} \varphi(B) d B
$$

The integral term in the flux expression can be calculated as, provided that a function with a denominator that may cancel out may be integrated (Abramowitz and Stegun 1972) ${ }^{32}$ :

$$
\int_{-1}^{+1} \frac{1}{\Sigma_{t}-i B \mu^{\prime}} d \mu^{\prime}=\frac{1}{i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)=\frac{2}{B} \operatorname{Arctan}\left(\frac{B}{\Sigma_{t}}\right)
$$

A similar solution is obtained by noting that the Dirac function is the Fourier transform of one:

$$
\delta(x)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{+i B x} d B
$$

The flux solution is sought by writing the equation under the following form:

$$
\Phi(x, \mu)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} \frac{f(B)}{\Sigma_{t}-i B \mu} e^{+i B x} d B
$$

The introduction of such an expression may not seem very natural, but it can be observed that the term $\Sigma_{t}(x)-i B \mu$ would appear if the Fourier transform was applied. Injecting these two expressions in the differential equation leads to an equation on $f(B)$ :

[^207]$$
f(B)=f(B) \frac{\Sigma_{s, 0}}{2} \int_{-1}^{+1} \frac{1}{\Sigma_{t}-i B \mu^{\prime}} d \mu^{\prime}+\frac{1}{2}
$$
which after integration leads to:
$$
f(B)=\frac{1}{2\left[1-\frac{\Sigma_{s, 0}}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)\right]}
$$

The integrated flux results from the integration over $\mu$ :

$$
\begin{aligned}
\Phi(x) & =\frac{1}{2 \pi} \int_{-1}^{+1} d \mu \int_{-\infty}^{+\infty} \frac{f(B)}{\Sigma_{t}(x)-i B \mu} e^{+i B x} d B \\
& =\frac{1}{4 \pi} \int_{-\infty}^{+\infty} \frac{1}{\left[1-\frac{\Sigma_{s, 0}}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)\right]} \frac{\ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)}{i B} e^{+i B x} d B
\end{aligned}
$$

Duderstadt and Martin (1979) analyzed Eq. (9.34) in the complex space by noting the role of the poles $\Sigma_{t} i$ and $-\Sigma_{t} i$, and proved that the complete result for the inverse transform is written as:

$$
\Phi(x)=a_{0} e^{-B_{0} x}+\int_{\Sigma_{T}}^{+\infty} S(B) e^{-B x} d B
$$

where $B_{0}$ is the root of:

$$
\begin{equation*}
\text { Compatibility condition: } 1-\frac{\Sigma_{s, 0}}{2 i B_{0}} \ln \left(\frac{\Sigma_{t}+i B_{0}}{\Sigma_{t}-i B_{0}}\right)=0 \tag{9.35}
\end{equation*}
$$

$$
\text { and } A(B)=\frac{1}{2 B\left[1-\frac{\Sigma_{s, 0}}{2 B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)+\left(\frac{\Sigma_{s, 0} \pi}{2 B}\right)^{2}\right]}
$$

This analysis implies that the flux is the sum of a transient flux which cancels out as the distance from the source increases, and an asymptotic flux towards which the flux tends ad infinitum.

Blaquière (1962) observed that only the terms in the neighborhood of the square root of $B_{0}$ contribute significantly to the flux $\Phi(x)$, thereby leading to a perturbation approach by setting: $B=B_{0}+\delta B$ and by taking the Taylor expansion of the term at the denominator along with the use of Eq. 9.35 , we obtain:

$$
\begin{aligned}
& \left\{\begin{array}{l}
1-\frac{\Sigma_{s, 0}}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)=1-\frac{\Sigma_{s, 0}}{2 i\left(B_{0}+\delta B\right)} \ln \left(\frac{\Sigma_{t}+i B_{0}}{\Sigma_{t}-i B_{0}}\right) \ln \left(\frac{1+\frac{i \delta B}{\Sigma_{t}+i B_{0}}}{1-\frac{i \delta B}{\Sigma_{t}-i B_{0}}}\right) \\
\approx 1-\frac{\Sigma_{s, 0}}{2 i B_{0}}\left(1+\frac{\delta B}{B_{0}}\right)\left[\ln \left(\frac{\Sigma_{t}+i B_{0}}{\Sigma_{t}-i B_{0}}\right)+\frac{i \delta B}{\Sigma_{t}+i B_{0}}-\frac{i \delta B}{\Sigma_{t}-i B_{0}}\right] \approx \frac{\delta B}{B_{0}}\left(1-\frac{\Sigma_{t} \Sigma_{s, 0}}{\Sigma_{t}^{2}+B_{0}^{2}}\right) \\
\text { and } \quad \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right) \approx \frac{2 i B_{0}}{\Sigma_{s, 0}}+\frac{2 i \Sigma_{t} \delta B}{\Sigma_{t}^{2}+B_{0}^{2}}
\end{array}\right.
\end{aligned}
$$

thus:

$$
\begin{aligned}
& \qquad(x)=\frac{1}{4 \pi} \int_{-\infty}^{+\infty} \frac{1}{\left[1-\frac{\Sigma_{s, 0}}{2 i B} \ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)\right]} \frac{\ln \left(\frac{\Sigma_{t}+i B}{\Sigma_{t}-i B}\right)}{i B} e^{+i B x} d B \\
& \\
& \approx \frac{1}{4 \pi} \int_{-\infty}^{+\infty} \frac{e^{+i B x}}{i \delta B\left(1-\frac{\Sigma_{t} \Sigma_{s, 0}}{\Sigma_{t}^{2}+B_{0}^{2}}\right)} \frac{2 i B_{0}}{\Sigma_{s, 0}} d B \\
& \text { i.e.: } \Phi(x)=
\end{aligned}
$$

The Fourier transform (Lavoine 1963) of:

$$
f(x)=\left\{\begin{array}{cc}
e^{-\frac{x}{a}} e^{i B_{0} x} & \text { for } x \geq 0 \\
0 & \text { for } x<0
\end{array} \quad \text { is } F(B)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i B x} f(x) d x=\frac{1}{i\left(B-B_{0}\right)+\frac{1}{a}}\right.
$$

This result is also reached (Oberhettinger 1973) by calculating the characteristic function $\varphi(t)=\int_{-\infty}^{+\infty} f(x) e^{i t x} d x$ that corresponds to the probability density $f(x)=$ $\frac{C^{p}}{\Gamma(p)} x^{p-1} e^{-C_{x}}$ and which is equal to $\varphi(t)=\frac{C^{p}}{(C-i t)^{p}}$. It means that the integral $\frac{1}{2 \pi} \int_{-\infty}^{+\infty} \frac{e^{+i B x}}{i\left(B-B_{0}\right)} d B$ is the inverse Fourier transform and is equal to $e^{i B_{0} x}$ by taking the limit as $a$ tends towards infinity. By setting $\kappa=-i B_{0}$, the asymptotic flux is thus written as:

$$
\Phi_{\text {asymptotic }}(x)=\frac{\kappa}{\Sigma_{s, 0}} \frac{1}{\left(\frac{\Sigma_{t} \Sigma_{s, 0}}{\Sigma_{t}^{2}+\kappa^{2}}-1\right)} e^{-\kappa x}
$$

It will be seen later on that the flux in diffusion theory can be expressed as:

$$
\Phi_{\text {diffusion }}(x)=\frac{\kappa}{2 \Sigma_{a}} e^{-\kappa x}
$$

As pointed out by Weinberg and Wigner (1958, p. 240), Blaquière (1962, p. 151) and Barjon (1993, p. 107), the diffusion flux is the asymptotic solution of the transport equation in a weakly absorbing medium and far from sources. The transport theory predicts a more significant absorption of neutrons close to the source. Equation (9.35) is written as follows with the new notations:

$$
-\frac{\Sigma_{s, 0}}{2 \kappa} \ln \left(\frac{\Sigma_{t}-\kappa}{\Sigma_{t}+\kappa}\right)=1
$$

i.e.:

$$
\frac{\kappa}{\Sigma_{t}}=\tanh \left(\frac{\kappa}{\Sigma_{s, 0}}\right) \approx \frac{\kappa}{\Sigma_{s, 0}}-\frac{1}{3}\left(\frac{\kappa}{\Sigma_{s, 0}}\right)^{3}+\frac{2}{15}\left(\frac{\kappa}{\Sigma_{s, 0}}\right)^{5}+\ldots
$$

thus

$$
\frac{1}{3} \frac{\kappa^{2}}{\Sigma_{s, 0}^{3}} \approx \frac{\Sigma_{t}-\Sigma_{s, 0}}{\Sigma_{t} \Sigma_{s, 0}}=\frac{\Sigma_{a}}{\Sigma_{t} \Sigma_{s, 0}}
$$

and, finally, in a medium where $\Sigma_{a} \approx \Sigma_{s, 0}$ :

$$
\kappa \approx \sqrt{3 \Sigma_{a} \Sigma_{s, 0}}
$$

It will be seen later on that the quantity $\kappa$, which has the dimensions of the inverse of a length, corresponds to the inverse of the scattering distance in diffusion theory. The previous derivations included complex numbers. Real functions are employed by seeking the flux as a decaying exponential function in space:

$$
\Phi(x)=\Phi_{0} e^{-\kappa x}
$$

Furthermore, the space and angle variables will be assumed to be separable as:

$$
\Phi(x, \mu)=\varphi(\mu) e^{-\kappa x}
$$

Such a factorized flux satisfies the Boltzmann equation in a homogeneous medium without sources and is called the relaxation mode. The flux and the scattering cross sections are expanded with Legendre polynomials, and the angular part of the flux is written as:

$$
-\mu \kappa \varphi(\mu)+\Sigma_{t} \varphi(\mu)=\frac{1}{2} \sum_{l=0}^{n}(2 l+1) \Sigma_{s, l} P_{l}(\mu) \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) P_{l}\left(\mu^{\prime}\right) d \mu^{\prime}
$$

Hence, $\varphi(\mu)$ is written as:

$$
\varphi(\mu)=\frac{1}{2} \sum_{l=0}^{n}(2 l+1) \frac{\Sigma_{s, l} P_{l}(\mu)}{\Sigma_{t}-\mu \kappa} \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) P_{l}\left(\mu^{\prime}\right) d \mu^{\prime}
$$

The angular moments $\varphi_{l} \int_{-1}^{+1} \varphi\left(\mu^{\prime}\right) P_{l}\left(\mu^{\prime}\right) d \mu^{\prime}$ are obtained by multiplying the previous equation by $P_{l}(\mu)$, and then integrating over $[-1,+1]$. Usually, this technique is employed to benefit from the orthogonality relations of the Legendre polynomials. However, the term $\Sigma_{t}-\mu \kappa$ in the denominator leads to the following coefficients:

$$
g_{k l}(\alpha)=g_{l k}(\alpha)=\int_{-1}^{+1} \frac{P_{k}(\mu) P_{l}(\mu)}{1-\mu \alpha} d \mu \quad \text { with } \alpha=\frac{\kappa}{\Sigma_{t}}
$$

for which the first terms are easily computed as:

$$
\left\{\begin{array}{l}
g_{00}(\alpha)=\int_{-1}^{+1} \frac{1}{1-\mu \alpha} d \mu=\frac{1}{\alpha} \ln \frac{1+\alpha}{1-\alpha} \\
g_{10}(\alpha)=\int_{-1}^{+1} \frac{\mu}{1-\mu \alpha} d \mu=\frac{1}{\alpha^{2}}\left[\ln \frac{1+\alpha}{1-\alpha}-2 \alpha\right] \\
g_{11}(\alpha)=\int_{-1}^{+1} \frac{\mu^{2}}{1-\mu \alpha} d \mu=\frac{1}{\alpha^{3}}\left[\ln \frac{1+\alpha}{1-\alpha}-2 \alpha\right] \\
g_{20}(\alpha)=\int_{-1}^{+1} \frac{\frac{1}{2}\left(3 \mu^{2}-1\right)}{1-\mu \alpha} d \mu=\frac{3}{2} g_{10}(\alpha)-\frac{1}{2} g_{00}(\alpha)
\end{array}\right.
$$

Therefore, a linear system of equations for the angular flux moments is reached:

$$
\left\{\begin{array}{l}
\varphi_{0}=\frac{1}{2 \Sigma_{t}}\left[\Sigma_{s, 0} g_{00}(\alpha) \varphi_{0}+3 \Sigma_{s, 1} g_{01}(\alpha) \varphi_{1}+5 \Sigma_{s, 2} g_{02}(\alpha) \varphi_{2}+\ldots \ldots\right] \\
\varphi_{0}=\frac{1}{2 \Sigma_{t}}\left[\Sigma_{s, 0} g_{10}(\alpha) \varphi_{0}+3 \Sigma_{s, 1} g_{11}(\alpha) \varphi_{1}+5 \Sigma_{s, 2} g_{12}(\alpha) \varphi_{2}+\ldots \ldots\right] \\
\ldots .
\end{array}\right.
$$

These equations can be generalized as:

$$
\varphi_{k}=\frac{1}{2 \Sigma_{t}} \sum_{l=0}^{n}(2 l+1) \Sigma_{s, l} g_{l k}(\alpha) \varphi_{l} \quad \text { for } k=1, n
$$

In $B_{1}$ approximation, the expansion is limited to order 1. Recent developments in the $B_{n}$ method (consistent $B_{n}$ method ${ }^{33}$ ) allow for anisotropic collision probability that accounts for periodic boundary conditions directly in the uncollided flux calculation in plane geometry. They have shown the microscopic flux of a lattice of slabs can be calculated without any restriction on the anisotropy order of the collision law.

[^208]
## $9.11 T_{n}$ Method



Pafnuty Chebyshev (1821-1894), Russian mathematician who taught Markov and Lyapunov (Public domain)

The $T_{n}$ method consists in expanding both the flux and the scattering cross section on the basis of Chebyshev polynomials of the first kind. This method is fairly interesting given that the Chebyshev polynomials best approximate a function in the Von Neumann minimax sense whereas the Legendre polynomials do so in the least square sense. It implies that the use of Chebyshev polynomials leads to errors which are equally distributed on the $[-1,1]$ range of the cosine of the scattering angle, whereas the error due to Legendre polynomials is maximum for $\mu=1$ or -1 . This analysis is essential as there is significant oscillation effects due to polynomials as their orders are increased to match a given function. Such oscillations may cause problems for incident or outgoing directions. The expression of Chebyshev polynomials is given by $T_{n}\left(\cos \theta_{0}\right)=\cos \left(n \theta_{0}\right)$, the first few terms being given below:

$$
\left\{\begin{array}{cc}
T_{0}(\mu)=1 & T_{3}(\mu)=4 \mu^{3}-3 \mu \\
T_{1}(\mu)=\mu & T_{4}(\mu)=8 \mu^{4}-8 \mu^{2}+1 \\
T_{2}(\mu)=2 \mu^{2}-1 & T_{5}(\mu)=16 \mu^{5}-20 \mu^{3}+5 \mu
\end{array}\right.
$$

with the orthogonality property written as:

$$
\int_{-1}^{+1} \frac{T_{n}(\mu) T_{m}(\mu)}{\sqrt{1-\mu^{2}}} d \mu= \begin{cases}0 & \text { if } n \neq m \\ \pi & \text { if } n=m=0 \\ \frac{\pi}{2} & \text { if } n=m \neq 0\end{cases}
$$

The Chebyshev polynomials satisfy the following recurrence relation:

$$
T_{n+2}(\mu)+T_{n}(\mu)-2 \mu T_{n+1}(\mu)=0
$$

There is a strong similarity with the $P_{n}$ approach since an addition formula also exists ${ }^{34}$ such that a polynomial in $\mu_{0}$ can be expanded in $\mu$ and $\mu^{\prime}$ as shown by:

$$
\begin{aligned}
T_{n}\left(\mu_{0}\right)= & \sum_{m=0}^{n} \sum_{i=0}^{E[(n-m) / 2]} \sum_{j=0}^{E[(n-m) / 2]} \sum_{k=0}^{E[(n-m) / 2]} t_{i, j, k}^{n, m} \sin ^{m}(\varphi) \sin ^{m}\left(\varphi^{\prime}\right) T_{n-m-2 i}(\mu) \\
& \times T_{n-m-2 j}\left(\mu^{\prime}\right) \times T_{n-m-2 k}\left(\cos \left(\varphi-\varphi^{\prime}\right)\right)
\end{aligned}
$$

where the coefficient $t_{i, j, k}^{n, m}$ is equal to:

$$
t_{i, j, k}^{n, m}=\left\{\begin{array}{l}
1 \quad \text { if } n=0 \\
\frac{n}{\pi} \quad 4(n-m)!\left(\frac{1}{2}-m\right) \Gamma(i+m) \Gamma(n-i) \Gamma(j+m) \Gamma(n-j) \Gamma\left(k-\frac{1}{2}\right) \Gamma\left(m-k-\frac{1}{2}\right) \\
\pi \Gamma+m) \Gamma(m) \Gamma(m) \Gamma(i+1) \Gamma(n-m-i+1) \Gamma(j+1) \Gamma(n-m-j+1) \Gamma(k+1) \Gamma(n-k+1) \\
\quad \times\left(1-\frac{1}{2} \delta_{2 i, n-m}\right)\left(1-\frac{1}{2} \delta_{2 j, n-m}\right)\left(1-\frac{1}{2} \delta_{2 k, m}\right) \text { for } n>0
\end{array}\right.
$$

where $\Gamma(x)$ is the usual real factorial. The Chebyshev polynomials are projections of the ultraspherical harmonic functions $C_{n}^{\alpha}$ also known as the Gegenbauer polynomials (Abramovitz and Stegun 1972; Robin 1959, p. 183), just like the Legendre polynomials are projections of the spherical harmonics. The complex nature of the algebraic formulae is due to the fact that few developments have been undertaken in this field compared to the widespread use of spherical harmonics, as underlined by Milgram. Let us consider the expansion of the flux and the scattering cross section as Chebyshev series:

$$
\Phi(x, \mu)=\sum_{l=0}^{\infty} \varphi_{l}(x) T_{l}(\mu) \quad \text { and } \quad \Sigma_{s}\left(x, \mu_{0}\right)=\sum_{n=0}^{n} \Sigma_{l}(x) T_{l}\left(\mu_{0}\right)
$$

which are injected in the $l D$ transport equation in its monoenergetic form for simplifications:
$\mu \frac{\partial \Phi(x, \mu)}{\partial x}+\Sigma_{t} \Phi(x, \mu)=\frac{1}{4 \pi}\left[\int_{0}^{2 \pi} d \varphi \int_{-1}^{+1} \Sigma_{s}\left(x, \mu^{\prime}\right) \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}+\nu \Sigma_{f}(x) \int_{0}^{2 \pi} d \varphi \int_{-1}^{+1} \Phi\left(x, \mu^{\prime}\right) d \mu^{\prime}\right]$
Using the addition formula, the following equation is reached:

[^209]\[

$$
\begin{aligned}
& \sum_{l}\left[\mu \frac{\partial \phi_{l}(x)}{\partial x}+\Sigma_{t} \phi_{l}(x)\right] T_{l}(\mu)=\sum_{l=0}^{n} \Sigma_{l}(x) \sum_{m=0}^{l} \sum_{i=0}^{E[l-m) / 2]} \sum_{j=0}^{E[l-m) / 2]} \sum_{k=0}^{E[m / 2]} t_{i, j, k}^{n, m} T_{l-m-2 i}(\mu) \\
& \times \sum_{p} \phi_{p}(x) \sin ^{m} \theta \gamma_{l-m-2 j, p, m} \beta_{m-2 k}+\nu \Sigma_{f} \sum_{l} \xi_{l, 0} \phi_{l}(x) \\
& \\
& \text { with }\left\{\begin{array}{l}
\gamma_{i, j, k}=\frac{1}{2} \int_{-1}^{+1} T_{i}\left(\mu^{\prime}\right) T_{j}\left(\mu^{\prime}\right) \sin ^{k}\left(\theta^{\prime}\right) d \mu^{\prime}=\frac{1}{2}\left(\xi_{i+j, k}+\xi_{|i-j|, k}\right) \\
\beta_{m}=\frac{1}{2 \pi} \int_{-1}^{+1} T_{m}\left(\cos \left(\varphi-\phi^{\prime}\right)\right) d \phi^{\prime}=\delta_{m, 0} \\
\xi_{l, m}=0 \quad \text { if } l \text { isodd }
\end{array}\right. \\
& \text { and }\left\{\begin{array}{l}
\xi_{l, m}=\frac{(-1)^{\frac{l}{2}} \Gamma\left(\frac{3}{2}\right) \Gamma\left(1+\frac{m}{2}\right) \Gamma\left(\frac{3}{2}+\frac{m}{2}\right)}{\Gamma\left(\frac{3}{2}+\frac{m}{2}-\frac{l}{2}\right) \Gamma\left(\frac{3}{2}+\frac{m}{2}+\frac{l}{2}\right)} \quad \text { if } l \text { is even } \\
\xi_{l, 0}=\frac{1}{1-l^{2}}
\end{array}\right.
\end{aligned}
$$
\]

The fact that $\beta_{m}=\delta_{m, 0}$ means that there are only even powers of $\sin \theta$, and thus, the higher degrees of $\sin ^{2} \theta \equiv 1-\mu^{2}$ may be employed to obtain $\mu^{2}=\left(T_{2}(\mu)+1\right) / 2$. Using the recurrence relation, the following equation is obtained:

$$
\mu^{m} T_{n}(\mu)=\frac{1}{2^{m}} \sum_{p=0}^{m} C_{n}^{p} T_{|n+m-2 p|}(\mu)
$$

Finally, the coefficients of the Chebyshev polynomials are obtained by inspection of each term (which is equivalent to the use of the orthogonality relation by multiplying the equation by $T_{l}(\mu) / \sqrt{1-\mu^{2}}$ and then integrating over [ $-1,+1$ ]) so as to obtain a system of coupled equations in $\phi_{l}(x)$ to the order $n$ :

$$
T_{n} \text { method: }\left\{\begin{array}{l}
\frac{1}{2}\left[\frac{\partial \varphi_{m}(x)}{\partial x}+\left(1+\delta_{m, 1}\right) \varphi_{m-2}(x)\right]=\sum_{k=0}^{n} \varphi_{m}(x) \sum_{j=k-2}^{n} A_{k, j} \Sigma_{s, j}  \tag{9.36}\\
\varphi_{-1}(x)=0 \quad \Sigma_{s,-1}=\Sigma_{t} \\
\varphi_{-2}(x)=0 \quad \Sigma_{s,-2}=\nu \Sigma_{f}
\end{array}\right.
$$

Milgram proposed the extension of the notations with negative indices to allow for a similar expansion of the fission source as that of the slowing-down source in the equation system. In 1989, Milgram calculated the first eight equations and provided the coefficients $A_{k, j}$ of the matrix. It should nevertheless be pointed out that this method which couples the flux moments of order $m$ and $m-2$ with all the others, leads to a denser matrix than the method for which the matrix is tri-diagonal
in $l D$, thereby implying that there will be an optimum in the precision to calculation cost ratio that is hard to appreciate at present. In a general approach, the Gegenbauer ultrasphercial functions $C_{n}^{\alpha}$ (for which the Chebyshev polynomials are degenerate as $\alpha \rightarrow 0$ ) can be directly employed at the expense of higher computational costs and the use of symbolic calculators to evaluate the matrix coefficients.

## $9.12 \quad F_{n}$ Method

The $F_{n}{ }^{35}$ method consists in expanding the flux on the following basis functions:

$$
\Phi(r, \mu)=\mu^{2} \sum_{l=0}^{n} \varphi_{l}(r) P_{l}^{*}(\mu)
$$

where $P_{l}^{*}(\mu)$ is the shifted Legendre polynomial $P_{l}(2 \mu-1)$ which was previously discussed in Yvon's method $\left(D P_{n}\right)$. The transport current of such an expansion is given as:

$$
J(r)=\mu^{2} \sum_{l=0}^{n} \frac{d \varphi_{l}(r)}{d r} \int_{0}^{1} \mu^{2} P_{l}^{*}(\mu) d \mu=\frac{1}{3} \frac{d \varphi_{0}(r)}{d r}+\frac{1}{30} \frac{d \varphi_{2}(r)}{d r}
$$

Such an expansion is particularly interesting for transport calculations in cylindrical geometries.

## $9.13 C_{n}$ Method

The $C_{n}$ method (based on the Complementarity theory, thus the $C$ in the name) is an original method developed at CEA Saclay by Pierre Benoist and Alain Kavenoky on the basis of the third form of the transport equation. This method consists in expanding the flux $\Phi(\mu)$ and the adjoint flux $\Phi^{*}(\mu)$ on a polynomial basis over the $[0,1]$ range. Let us expand the Milne problem example discussed in Chap. 8, as in the PhD work of Alain Kavenoky. The equations at the interface of a medium and vacuum were established for an incident flux $\Phi^{+}(\mu)$ :

[^210]\[

\left\{$$
\begin{array}{l}
0=\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}+\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \quad \text { for } \mu>0 \\
\Phi^{+}(\mu)=\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}+\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) G_{m c}\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \quad \text { for } \mu<0
\end{array}
$$\right.
\]

These two equations can be written in the canonical form of an integral Fredholm equation with a symmetric kernel by posing the intermediate function $f$ $(\mu)=\sqrt{\mu} \Phi^{-}(-\mu)$ for $\mu>0$ :

$$
\left\{\begin{array}{l}
\underbrace{\sqrt{\mu} \int_{0}^{1} \int_{\mu^{\prime} \Phi^{+}}\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) d \mu^{\prime}}_{S_{1}(\mu)}-\int_{0}^{1} f\left(\mu^{\prime}\right) H_{1}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}=0, \quad H_{1}\left(\mu^{\prime}, \mu\right)=\sqrt{\mu \mu^{\prime}} G\left(-\mu^{\prime}, \mu\right) \\
\underbrace{\sqrt{\mu} \int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) G\left(\mu^{\prime},-\mu\right) d \mu^{\prime}}_{s_{2}(\mu)}-\int_{0}^{1} f\left(\mu^{\prime}\right) H_{2}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}=0, \quad H_{2}\left(\mu^{\prime}, \mu\right)=\delta\left(\mu-\mu^{\prime}\right)+\sqrt{\mu \mu^{\prime}} G\left(\mu^{\prime}, \mu\right)
\end{array}\right.
$$

This canonical form allows the use of a myriad of appropriate mathematical methods for a symmetrical kernel. The albedo can be calculated as the ratio of the outgoing current to the incoming current:

$$
\beta \equiv \frac{\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) d \mu^{\prime}}{\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) d \mu^{\prime}}=\frac{\int_{0}^{1} \sqrt{\mu^{\prime}} f\left(\mu^{\prime}\right) d \mu^{\prime}}{\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) d \mu^{\prime}}
$$

Normalizing the current to one $\int_{0}^{1} \mu^{\prime} \Phi^{+}\left(\mu^{\prime}\right) d \mu^{\prime}=1$ leads to:

$$
\beta=\int_{0}^{1} \sqrt{\mu^{\prime}} f\left(\mu^{\prime}\right) d \mu^{\prime}=-\int_{-1}^{0} \mu^{\prime} \Phi^{-}\left(\mu^{\prime}\right) d \mu^{\prime}
$$

The adjoint equation to Eq. (9.37) is defined wrt the albedo:

$$
\begin{equation*}
\sqrt{\mu}-\int_{0}^{1} f^{*}\left(\mu^{\prime}\right) H_{i}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}=0 \quad i=1 \text { or } 2, \mu>0 \tag{9.38}
\end{equation*}
$$

The adjoint property is satisfied by the fact that:

$$
\forall i, \quad \begin{aligned}
\int_{0}^{1} f^{*}(\mu) S_{i}(\mu) d \mu & =\int_{0}^{1} f^{*}(\mu) d \mu \int_{0}^{1} f\left(\mu^{\prime}\right) H_{i}\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \\
& =\int_{0}^{1} f\left(\mu^{\prime}\right) d \mu^{\prime} \int_{0}^{1} f^{*}(\mu) \underbrace{H_{i}\left(\mu^{\prime}, \mu\right)}_{=H_{i}\left(\mu \mu^{\prime}\right)} d \mu^{\prime}=\int_{0}^{1} f\left(\mu^{\prime}\right) \sqrt{\mu^{\prime}} d \mu^{\prime}=\beta
\end{aligned}
$$

The adjoint function $f^{*}(\mu)$ defines $\Phi^{*}(\mu)$ as: $f^{*}(\mu) \equiv \sqrt{\mu} \Phi^{*}(-\mu) \quad \mu>0$.
In 1952, Kahan ${ }^{36}$ and Rideau showed ${ }^{37}$ that the stationary nature of the bilinear functional:

Kahan-Rideau functional: $\beta\left(f, f^{*}\right) \equiv \int_{0}^{1} f(\mu) \sqrt{\mu} d \mu+\int_{0}^{1} f^{*}(\mu) S_{i}(\mu) d \mu$

$$
\begin{equation*}
-\int_{0}^{1} f^{*}(\mu) d \mu \int_{0}^{1} f\left(\mu^{\prime}\right) H_{i}\left(\mu^{\prime}, \mu\right) d \mu^{\prime} \tag{9.39}
\end{equation*}
$$

implied that the functions $f(\mu)$ and $f^{*}(\mu)$ were solutions to Eqs. (9.37) and (9.38) respectively. In fact:

$$
\begin{aligned}
\delta \beta\left(f, f^{*}\right) \equiv & \int_{0}^{1} \delta f^{*}(\mu) d \mu\left(S_{i}(\mu)-\int_{0}^{1} f\left(\mu^{\prime}\right) H_{i}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}\right) \\
& +\int_{0}^{1} \delta f(\mu) d \mu\left(\sqrt{\mu}-\int_{0}^{1} f^{*}\left(\mu^{\prime}\right) H_{i}\left(\mu^{\prime}, \mu\right) d \mu^{\prime}\right)
\end{aligned}
$$

[^211]
## MEMORIAL

## ozs <br> SCIENCES MATHÉMATIOUES

##  <br> L'ACADÉMIE DES SCIENCES DE PARIS,




## dinkgtegn,

Henfi villat
Hebtoc or ricedem


fascicule cxxxiv

## Les méthodes d'approximation variatiomelles

 dans la theorie des collisions atomiques et dans la physique des piles nucléairesPar mm. t. kahan, g. rideau et P. roussopoulos


PARIS
GAUTHIER-VILLARS, EDITEUR-IMPRIMEUR-LIBRAIRE
Quai des Grands-Augatins, 55

## 1956

The works of Kahan and Rideau on the variational approximation applied to neutron physics are grouped in this memorial of mathematical sciences, fascicle CXXXIV of 1956 (The Marguet collection)

By substituting the definitions of $f(\mu), f^{*}(\mu)$ and $H_{i}\left(\mu^{\prime}, \mu\right)$, the following equation is obtained for the first expression:

$$
\begin{aligned}
\beta\left(\Phi, \Phi^{*}\right) \equiv & -\int_{-1}^{0} \Phi(\mu) \mu d \mu-\int_{-1}^{0} \Phi^{*}(\mu) \mu d \mu \int_{0}^{1} \Phi^{+}\left(\mu^{\prime}\right) G\left(\mu^{\prime},-\mu\right) \mu^{\prime} d \mu^{\prime} \\
& -\int_{-1}^{0} \Phi^{*}(\mu) \mu d \mu \int_{-1}^{0} \Phi\left(\mu^{\prime}\right) G\left(\mu^{\prime},-\mu\right) \mu^{\prime} d \mu^{\prime}
\end{aligned}
$$

and for the second one:

$$
\begin{aligned}
\beta\left(\Phi, \Phi^{*}\right) \equiv & -\int_{-1}^{0} \mu d \mu-\int_{-1}^{0} \Phi^{*}(\mu) \mu d \mu \int_{0}^{1} \Phi^{+}\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) \mu^{\prime} d \mu^{\prime} \\
& +\int_{-1}^{0} \Phi^{*}(\mu) \mu d \mu-\int_{-1}^{0} \Phi^{*}(\mu) \mu d \mu \int_{-1}^{0} \Phi\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) \mu^{\prime} d \mu^{\prime}
\end{aligned}
$$

The $C_{n}$ approximation consists in expanding ${ }^{38}$ :

$$
\Phi(\mu)=\sum_{l=0}^{n} \Phi_{l} \mu^{l} \quad \text { and } \quad \Phi^{*}(\mu)=\sum_{l=0}^{n} \Phi_{l}^{*} \mu^{l}
$$

These expressions are injected in the Kahan-Rideau functional, and the stationary conditions are sought by cancelling the derivatives wrt $\Phi_{l}$ and $\Phi_{l}^{*}$. For a $C_{0}$ expansion where the angular fluxes are constant: $\Phi(\mu)=\Phi_{0}$ and $\Phi^{*}(\mu)=\Phi_{0}^{*}$, and for both formulations, we obtain the following equations:

$$
\left\{\begin{array}{l}
\beta_{0}^{1}=-\frac{1}{2} \frac{\int_{0}^{1} \mu d \mu \int_{0}^{1} \Phi^{+}\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) \mu^{\prime} d \mu}{\int_{0}^{1} \mu d \mu \int_{-1}^{0} G\left(\mu^{\prime}, \mu\right) \mu^{\prime} d \mu} \\
\beta_{0}^{2}=-\frac{1}{2} \frac{\int_{0}^{0} \mu d \mu \int_{0}^{1} \Phi^{+}\left(\mu^{\prime}\right) G\left(\mu^{\prime}, \mu\right) \mu^{\prime} d \mu}{\frac{1}{2}+\int_{0}^{1} \mu d \mu \int_{0}^{1} G\left(\mu^{\prime}, \mu\right) \mu^{\prime} d \mu}
\end{array}\right.
$$

It is recalled that $\Phi^{+}(\mu)$ is an input data in the Milne problem and that the terms in the denominator contain the first moment of the Green function in infinite medium, that are easily computed. A $C_{n}$ approximation leads to more complicated expressions with higher moments of the Green function.

[^212]The $C_{n}$ method proved to be as precise as, or even more, than the collision probability method, especially for $l D$ problems where the Green function is easily calculated analytically, and where the method, which deals with interface flux, is independent of the size of the cells in the mesh. It was successfully applied by Henri Lorain ${ }^{39,40,41}$ to deal with the exponential experiments where a neutron source is applied to one face of a parallelepiped to measure its neutronic properties.

### 9.14 The $S K_{n}$ Method

The $S K_{n}$ method stems from the approach of M. Krook ${ }^{42}$ for radiative transfer (1955). The idea was applied to neutron physics by Bernard Spinrad and J. Sterbentz ${ }^{43,44}$ and consists in expanding the exponential term which appears in the specific-volume form of the integral Boltzmann equation (expressed here for isotropic scattering and source, and a homogeneous medium):

$$
\Phi(\vec{r})=\int_{V} d^{3} r^{\prime} \frac{e^{-\Sigma_{t}\left|\vec{r}-\vec{r}^{\prime}\right|}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}}\left(\Sigma_{s, 0}\left(\vec{r}^{\prime}\right) \Phi\left(\vec{r}^{\prime}\right)+S\left(\vec{r}^{\prime}\right)\right)
$$

The exponential expansion is carried out through the exponential integral term:

$$
e^{-x}=x E_{0}(x)=x \int_{0}^{1} \frac{e^{-\frac{x}{\mu}}}{\mu^{2}} d \mu \approx x \sum_{l=1}^{n} \frac{\omega_{l}}{\mu_{l}^{2}} e^{-\frac{x}{\mu_{l}}}
$$

The weights $\omega_{l}$ and $\mu_{l}$ are chosen such that they satisfy:

[^213]$$
\int_{0}^{+\infty} x^{k} e^{-x} d x=\Gamma(k+1)=\sum_{l=1}^{n} \frac{\omega_{l}}{\mu_{l}^{2}} \int_{0}^{+\infty} x^{k+1} e^{-\frac{x}{\mu_{l}}} d x \quad \text { for } k=0 \text { to } 2 n-1
$$
$\omega_{l}$ and $\mu_{l}$ are the weights of the Gauss quadrature for the integral $E_{0}(x)$. The exponential term of the uncollided flux kernel is written as follows with these assumptions:
$$
e^{-\Sigma_{l}\left|\vec{r}-\vec{r}^{\prime}\right|} \approx \sum_{l=1}^{n} \frac{\omega_{l}}{\mu_{l}^{2}} \Sigma_{t}\left|\vec{r}-\vec{r}^{\prime}\right| e^{-\frac{\Sigma_{l}\left|\vec{r}-\vec{r}^{\prime}\right|}{\mu_{l}}}
$$

The integral equation can hence be written under the following form:

$$
\begin{gathered}
\Phi(\vec{r})=\int_{V} d^{3} r^{\prime} \frac{\sum_{=1}^{n} \frac{\omega_{l}}{\mu_{l}^{2}} \sum_{t}\left|\vec{r}-\vec{r}^{\prime}\right| e^{-\frac{\Sigma_{l}\left|\vec{r}-\vec{r}^{\prime}\right|}{\mu_{l}}}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}} \underbrace{\left(\Sigma_{s, 0}\left(\vec{r}^{\prime}\right) \Phi\left(\vec{r}^{\prime}\right)+S\left(\vec{r}^{\prime}\right)\right)}_{q\left(\vec{r}^{\prime}\right)} \equiv \sum_{l=1}^{n} \omega_{l} \Phi_{l}(\vec{r}) \\
\text { with: } \quad \Phi_{l}(\vec{r}) \equiv \frac{1}{D_{l}} \int_{V} d^{3} r^{\prime} \frac{\sum_{l=1}^{n} e^{-\frac{\Sigma_{l}\left|\overrightarrow{r_{-}}-\vec{l}^{\prime}\right|}{\mu_{l}}}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|} q\left(\vec{r}^{\prime}\right) \quad \text { and } \quad D_{l} \equiv \frac{\mu_{l}^{2}}{\Sigma_{t}}
\end{gathered}
$$

Each flux moment $\Phi_{l}(\vec{r})$ satisfies a diffusion equation such as:

$$
-D_{l} \Delta \Phi_{l}(\vec{r})+\Sigma_{t} \Phi_{l}(\vec{r})=q(\vec{r})
$$

The $S K_{n}$ equations are then expressed as:

$$
-D_{l} \Delta \Phi_{l}(\vec{r})+\Sigma_{t} \Phi_{l}(\vec{r})=\Sigma_{s} \sum_{m=1}^{n} \omega_{m} \Phi_{m}(\vec{r})+S(\vec{r})
$$

Hence, the same number of diffusion equations as the number of moments must be solved and carried out with a usual diffusion code, whilst the flux reconstruction in transport theory is executed outside that diffusion code. This method is very competitive even for heterogeneous problems using a wise implementation ${ }^{45}$ which is initially applied to homogeneous problems: a fictitious scattering term is added only along axis of the incident neutron (which cannot be discerned physically if there is no scattering) such that the total cross section becomes constant, and the optical path in the collisionless kernel is simplified.

[^214]
### 9.15 Method of Characteristics (MOC)

(Advances Nuclear Science and Technology, vol. 12, p. 1, 1980).

### 9.15.1 Principle

The Method of Characteristics consists in discretizing the transport equation in several directions such that the angular flux is approximated by a balance equation along a "tube" associated to a trajectory $T$. In practice, the angular flux is discretized by piecewise constant expansion by factorizing the space and angular direction variables:

Flux expansion in the method of characteristics: $\Phi(\vec{r}, \vec{\Omega}) \approx \sum_{i} \varphi_{i}(\vec{\Omega}) \psi_{i}(\vec{r})$
$\psi_{i}(\vec{r})$ is called the characteristic function of region $i$. Given a direction $\vec{\Omega}$, the flux in that direction may be expressed in integral form as:

$$
\Phi(\vec{r}, \vec{\Omega})=\Phi(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}) e^{-\overline{\Sigma_{t} \ell}(\vec{r}-\ell \vec{\Omega})}+\int_{0}^{\ell} q\left(\vec{r}-\ell^{\prime} \vec{\Omega}, \vec{\Omega}\right) e^{-\overline{\Sigma_{t} \ell}\left(\vec{r}-\ell^{\prime} \vec{\Omega}\right)} d \ell^{\prime}
$$

where the usual optical path discussed in the chapter on the Boltzmann equation is used:

$$
\overline{\Sigma_{t} \ell}(\vec{r}-\ell \vec{\Omega}) \equiv \int_{0}^{\ell} \Sigma_{t}\left(\vec{r}-\ell^{\prime} \vec{\Omega}\right) d \ell^{\prime}
$$

If the cross section is constant in the medium, the optical path is simplified as: $e^{-\Sigma_{t, i} \ell}$. If the collision kernel and the sources are zero, the exponential attenuation law of a collimated neutron beam in a given direction is obtained:

$$
\Phi(\vec{r}, \vec{\Omega})=\Phi(\vec{r}-\ell \vec{\Omega}, \vec{\Omega}) e^{-\Sigma_{t, i} \ell}
$$

Furthermore, in the extreme case where the total cross section is zero (which is the case of vacuum), the neutron flux in a direction does not change:
$\Phi(\vec{r}, \vec{\Omega})=\Phi(\vec{r}-\ell \vec{\Omega}, \vec{\Omega})$. The outgoing flux $\Phi^{\text {out }}(\vec{r}, \vec{\Omega})$ of a medium at position $\vec{r}$ can be calculated from the incoming flux using the transmission equation and the incoming flux $\Phi^{i n}(\vec{r}, \vec{\Omega})$ and the inner constant sources of medium $i$ by integrating the integro-differential equation along curvilinear coordinate $\ell$, with $\overrightarrow{r_{i n}}$ being the incident constant position for integration:

$$
\frac{\partial \Phi}{\partial \ell}=\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi\left(\overrightarrow{r_{i n}}+\ell \vec{\Omega}, \vec{\Omega}\right)=q_{i}(\vec{\Omega})-\Sigma_{t, i} \Phi\left(\overrightarrow{r_{i n}}+\ell \vec{\Omega}, \vec{\Omega}\right)
$$

i.e.:

Transmissionequation: $\Phi_{i}^{\text {out }}\left(\overrightarrow{r_{\text {out }}}, \vec{\Omega}\right)=\Phi_{i}^{\text {in }}(\vec{r}-L \vec{\Omega}, \vec{\Omega}) e^{-\Sigma_{t, i} L}+\frac{1-e^{-\Sigma_{t, i L}}}{\Sigma_{t, i}} q_{i}(\vec{\Omega})$

In this expression, $L$ is the length of the characteristic line that passes through medium $i$ and $\beta_{i}(\vec{r}, \vec{\Omega}) \equiv \frac{1-e^{-\Sigma_{t, i} L}}{\Sigma_{t, i}}$ is defined as the leakage probability in direction $\vec{\Omega}$.

A "tube" of length $L$ is associated to the direction $\vec{\Omega}$, as shown by Fig. 9.13, and is called a characteristic. The mean flux along a characteristic can be calculated by integrating the local flux along the path:

$$
\overline{\Phi_{L}}(\vec{\Omega})=\frac{1}{L} \int_{\ell=0}^{\ell=L} \Phi\left(\overrightarrow{r_{\text {in }}}+\ell \vec{\Omega}, \vec{\Omega}\right) d \ell=\frac{\Phi\left(\overrightarrow{r_{\text {out }}}, \vec{\Omega}\right)-\Phi\left(\overrightarrow{r_{\text {in }}}, \vec{\Omega}\right)}{\Sigma_{t, i} L}+\frac{q_{i}(\vec{\Omega})}{\Sigma_{t, i}}
$$

Integrating Eq. (9.41) on the volume of the cell (i.e. on all the tubes that pass through the cell $i$ in that direction, which is equivalent to the integration in the transverse direction of the axis of the tubes) leads to the usual balance equation:

Fig. 9.13 Path of a characteristic


$$
V_{i} \Sigma_{t, i} \varphi_{i}(\vec{\Omega})=V_{i} q_{i}(\vec{\Omega})+J_{i}^{\text {in }}(\vec{\Omega})-J_{i}^{\text {out }}(\vec{\Omega})
$$

The incoming and outgoing currents are given by:

$$
\begin{aligned}
J_{i}^{\text {in }}(\vec{\Omega})= & \int_{S_{i}^{\text {in } \left._{(\vec{\Omega}}\right)}} d S_{\text {in }} \vec{\Omega} \cdot \vec{n}_{\text {in }} \Phi_{\text {in }}(\vec{r}, \vec{\Omega}) \text { and } J_{i}^{\text {out }}(\vec{\Omega}) \\
& =\int_{S_{i}^{\text {out }}(\vec{\Omega})} d S_{\text {out }} \vec{\Omega} \cdot \vec{n}_{\text {out }} \Phi_{\text {out }}(\vec{r}, \vec{\Omega})
\end{aligned}
$$

Defining the transverse cross section of the tube as $S_{\oplus}$ and integrating over all the tubes, with $d S_{\text {in }}=S_{\oplus} / \vec{\Omega} \cdot \vec{n}_{\text {in }}$ and $d S_{\text {out }}=S_{\oplus} / \vec{\Omega} \cdot \vec{n}_{\text {out }}$, the following expressions are reached:

$$
J_{i}^{\text {in }}(\vec{\Omega})=\sum_{\text {trajectories }} S_{\oplus} \Phi_{\text {in }}(\vec{r}, \vec{\Omega}) \quad \text { and } \quad J_{i}^{\text {out }}(\vec{\Omega})=\sum_{\text {trajectories } \vec{\Omega}} S_{\oplus} \Phi_{\text {out }}(\vec{r}, \vec{\Omega})
$$

For paths of a given tube that are uniformly distributed, the cross section of the tubes is constant, and the angular flux is simply calculated by the balance equation as:

$$
\varphi_{i}(\vec{\Omega})=\frac{1}{\Sigma_{t, i}} q_{i}(\vec{\Omega})+\sum_{\text {trajectories }} \frac{S_{\oplus}\left[\Phi_{\text {in }}(\vec{r}, \vec{\Omega})-\Phi_{\text {out }}(\vec{r}, \vec{\Omega})\right]}{\Sigma_{t, i} V_{i}}
$$

### 9.15.2 Heterogeneous Geometries

The calculation of the integral in the transverse direction using the transverse cross section of tubes is equivalent to tracing equidistant rays and using the surface $S_{\oplus}$ as the weight in a quadrature formula which is the integration using the rectangle method. This is an essential point to be noted as numerical studies ${ }^{46}$ have shown that the global precision of the method of characteristics is limited by that of the transverse integration method. Each characteristic intercepts a given medium along

[^215]Fig. 9.14 Discretizing a lattice: The characteristic is at the center of the mesh cell, and indicated by an arrow

a series of segments for which the endpoints form a discrete set of points between which the regions are assumed to be homogeneous (Fig. 9.14).

For each segment, the transmission equation is applied and thus, information is propagated from the boundary conditions to edges of the complete geometry. The "distance travelled" along a characteristic, which includes a costly exponential calculation in the optical path, is called the sweep. For a given geometry, the segments are calculated only when the geometry is analyzed and it is quite remarkable that only the segment length is required for calculations. The angular flux is calculated by expressing the previous equation as:

$$
\varphi_{i}(\vec{\Omega})=\frac{1}{\Sigma_{t, i}}\left[1-\frac{1}{V_{i}} \sum_{\text {trajectories } \vec{\Omega}} S_{\oplus} \beta_{i}(\vec{r}, \vec{\Omega})\right] q_{i}(\vec{\Omega})+\sum_{\text {trajectories } \vec{\Omega}} \beta_{i}(\vec{r}, \vec{\Omega}) \varphi_{\text {in }}(\vec{\Omega})
$$

This form allows for the following iterative algorithm: the outgoing flux from a mesh cell is calculated for all the directions $\vec{\Omega}$ using the formula:

$$
\Phi_{i}^{\text {out }}(\vec{r}, \vec{\Omega})=\Phi_{i}^{\text {in }}(\vec{r}-\ell \vec{\Omega}, \vec{\Omega})+\beta_{i}(\vec{r}, \vec{\Omega})\left[q_{i}^{n-1}(\vec{\Omega})-\Sigma_{t, i} \Phi_{i}^{i n}(\vec{r}-\ell \vec{\Omega}, \vec{\Omega})\right]
$$

The outgoing flux terms are used to compute new values for $\Delta_{i}^{n}(\vec{\Omega})$ $=\sum_{\text {trajectories } \vec{\Omega}} \beta_{i}(\vec{r}, \vec{\Omega}) \varphi_{i n}(\vec{\Omega})$, which allows for the flux calculation at the new iteration:

$$
\varphi_{i}^{n}(\vec{\Omega})=\frac{1}{\Sigma_{t, i}}\left[1-\frac{1}{V_{i}} \sum_{\text {trajectories } \vec{\Omega}} S_{\oplus} \beta_{i}(\vec{r}, \vec{\Omega})\right] q_{i}(\vec{\Omega})+\Delta_{i}^{n}(\vec{\Omega})
$$

If the geometry is paved with homogeneous cells of volume $V_{j}$, a trajectory $T$ is the association of an angle $\vec{\Omega}$ and a starting point $\vec{p}$ chosen by scanning the perpendicular plane to direction $\vec{\Omega}$. These notations ${ }^{47}$ are practical for expressing the differential trajectory element as $d^{4} T=d^{2} \Omega d^{2} p$, the flux in the volume is thus calculated as:

$$
V_{j} \Phi_{j}=\int_{V_{j}} d^{3} r \int_{\Omega} d^{2} \Omega \Phi(\vec{r}, \vec{\Omega})=\int_{T} d^{4} T \int_{-\infty}^{+\infty} d \ell \delta\left(V_{j}, T\right) \Phi(\vec{p}+\ell \vec{\Omega})
$$

In this condensed expression, $\delta\left(V_{j}, T\right)$ is equal to 1 if the trajectory passes through the volume $V_{j}$, and 0 otherwise. A trajectory is a set of line segments $L_{k}$ between the starting point and the end point of each volume, i.e.:

$$
\overrightarrow{r_{k+1}}=\overrightarrow{r_{k}}-L_{k} \vec{\Omega}
$$

Roy points out that it is interesting to number these line segments in the inverse order of appearance in the trajectory for cyclic trajectories: $\left\{\cdots, L_{2}, L_{1}, L_{0}, L_{-1}\right.$, $\left.L_{-2} ; \cdots\right\}$. The mean flux along a segment is given by:

$$
L_{k} \overline{\Phi_{k}}(T)=\int_{\ell=0}^{\ell=L_{k}} \Phi\left(\overrightarrow{r_{k+1}}+\ell \vec{\Omega}, \vec{\Omega}\right) d \ell
$$

Hence:

$$
V_{j} \Phi_{j}=\int_{T} d^{4} T \sum_{k} \delta\left(V_{j}, L_{k}\right) L_{k} \overline{\Phi_{k}}(T)
$$

The same integration method can be applied for a volume that depends on the angle of the trajectory:

$$
V_{j}(\vec{\Omega})=\int_{p} d^{2} p \sum_{k} \delta\left(V_{j}, L_{k}\right) L_{k}
$$

[^216]If the paving of the domain into regions does not induce any preferential discretization such that this volume is an integer multiple of the volume of a tube, a renormalization of the optical path must be carried out such that the volume of the cell obtained by integration of the tubes is rigorously equal to the true volume. This process is carried out by substituting the integrated path $\ell$ of a tube by:

$$
\frac{V_{i}}{\sum_{\text {trajectories }} \underset{S_{\oplus}}{ } \ell(\text { trajectory })} \ell=\frac{V_{i}}{\int_{p} d^{2} p \sum_{k} \delta\left(V_{j}, L_{k}\right) L_{k}} \ell
$$

With these notations, the flux in the segment satisfies:

$$
\left\{\begin{array}{l}
\frac{d \Phi\left(\overrightarrow{r_{k+1}}+\ell \vec{\Omega}, \vec{\Omega}\right)}{d \ell}+\Sigma_{t, k} \Phi\left(\overrightarrow{r_{k+1}}+\ell \vec{\Omega}, \vec{\Omega}\right)=q_{k} \\
\Phi\left(\overrightarrow{r_{k+1}}+\ell \vec{\Omega}, \vec{\Omega}\right)=\Phi\left(\overrightarrow{r_{k+1}}, \vec{\Omega}\right) e^{-\Sigma_{t, k} \ell}+q_{k} \frac{1-e^{-\Sigma_{t, k} \ell}}{\Sigma_{t, k}}
\end{array}\right.
$$

The outgoing flux from the segment is:

$$
\Phi\left(\overrightarrow{r_{k}}, \vec{\Omega}\right)=\Phi\left(\overrightarrow{r_{k+1}}, \vec{\Omega}\right) e^{-\Sigma_{t, k} L_{k}}+q_{k} \frac{1-e^{-\Sigma_{t, k} L_{k}}}{\Sigma_{t, k}}
$$

and the angularly integrated flux is given by:

$$
\begin{aligned}
L_{k} \overline{\Phi_{k}}(T) & =\int_{\ell=0}^{\ell=L_{k}} \Phi\left(\overrightarrow{r_{k+1}}+\ell \vec{\Omega}, \vec{\Omega}\right) d \ell \\
& =\Phi\left(\overrightarrow{r_{k+1}}, \vec{\Omega}\right) \frac{1-e^{-\Sigma_{t, k} L_{k}}}{\Sigma_{t, k}}+\frac{q_{k}}{\Sigma_{t, k}}\left(L_{k}-\frac{1-e^{-\Sigma_{t, k} L_{k}}}{\Sigma_{t, k}}\right)
\end{aligned}
$$

Roy further notes that these expressions are finite when the medium is vacuum since:

$$
\lim _{\Sigma_{t, k} \rightarrow 0}\left(\frac{1-e^{-\Sigma_{t, k} L_{k}}}{\Sigma_{t, k}}\right)=L_{k} \quad \text { and } \quad \lim _{\Sigma_{t, k} \rightarrow 0} \frac{1}{\Sigma_{t, k}}\left(L_{k}-\frac{1-e^{-\Sigma_{t, k} L_{k}}}{\Sigma_{t, k}}\right)=\frac{L_{k}^{2}}{2}
$$

These equations are valid as long as the trajectory does not pass through a surface since the cross section of the medium is homogeneous. The balance equation is conserved for each cell in the mesh, the only approximation consists in assuming that the angular flux is piecewise-constant on the cell surface and that the volume-specific flux are constant per mesh cell, thereby requiring a wise spatial meshing. As for boundary conditions, applying void conditions at the boundary of convex domain ensures that neutrons cannot come back in the geometry, meaning that the trajectories stop at the outer boundary of a domain. The outgoing angular

Fig. 9.15 Example of a cyclic trajectory

flux are calculated after the sweeping of a characteristic but are not used afterwards since no neutron will contribute to the angular component of the current. However, if the trajectories cross reflective boundary conditions or translation/rotation conditions for cylindrical geometries, the outgoing angular flux at the intersection point of the characteristic/boundary is used over to calculate the incoming angular flux. This process is executed by the tracing of a "new" characteristic that satisfies the boundary conditions (Snell-Descartes law for specular reflection for instance, which reflects the trajectory by conserving the incident angle wrt the normal). Thus, the method becomes more complex given that the different directions are coupled to one another and cannot be traced independently. From a practical point of view, the neutron path is tracked until an open boundary is crossed, i.e void or a black body, which determines the last crossed region. The angular flux of that last region is directly injected in the appropriate region by sweeping the following segment of the current trajectory and keeping in mind, that all geometrical data are stored before the tracking is carried out. If the geometry is completely closed infinite trajectories are possible due to the boundary conditions. An approach ${ }^{48,49}$ consists in choosing cyclic trajectories for which it is ensured that they cross their starting points after a finite number of rebounds (Fig. 9.15).

Starting from a point $A$ and tracking a neutron through its successive reflections, it comes back to point $A$ again. At the first iteration, the incoming flux is not known and is assumed to be zero. Denoting $\Phi_{A}^{\text {in }}$ and $\Phi_{A}^{\text {out }}$ as the incoming and outgoing flux at point $A, \ell_{j}$ as the different segments of the trajectory, by applying the transmission equation, we obtain:

$$
\Phi_{A}^{\text {out }}=\Phi_{A}^{\text {in }} e^{-\sum_{j=1}^{N} \Sigma_{t, j} \ell_{j}}+\sum_{j=1}^{N} q_{j} e^{-\Sigma_{t, j} \ell_{j}}
$$

[^217]This formula is extended to the case of multiple media crossings by using the total length of the complete trajectory $L=\sum_{j=1}^{N} \ell_{j}$ and the optical path:

$$
\overline{\Sigma_{t} \ell}\left(\ell_{1}, \ell_{2}\right)=\int_{\ell=\ell_{1}}^{\ell=\ell_{2}} \Sigma_{t}(\ell) d \ell
$$

Hence:

$$
\Phi_{A}^{\text {out }}=\Phi_{A}^{\text {in }} e^{-\overline{\Sigma_{t} \ell}(0, L)}+\int_{\ell=0}^{\ell=L} q(\ell) e^{-\overline{\Sigma_{t} \ell}(\ell, L)} d \ell
$$

After a complete cycle of length $L$, the flux at point $A$ is obtained over again, and hence, $\Phi_{A}^{\text {out }}=\Phi_{A}^{i n}$. Therefore, the explicit calculation for that flux is:

$$
\Phi_{A}^{\text {in }}=\frac{\int_{\ell=0}^{\ell=L} q(\ell) e^{-\overline{\Sigma_{t} \ell}(\ell, L)}}{} d \ell
$$

Two successive sweeps of the trajectory are thus required to calculate all the flux at the intersection points of the complete trajectory with the boundaries. Ray-tracing techniques, very similar to $3 D$ imaging, have been employed to obtain high performance with the method of characteristics for heterogeneous media, especially as the method can be easily parallelized. Using the inverse indexing of segments as discussed earlier, the problem of crossing a surface described by an albedo can be simply substituted by a transmission equation:

$$
\Phi\left(\overrightarrow{r_{k}}, \vec{\Omega}\right)=\Phi\left(\overrightarrow{r_{k+1}}, \vec{\Omega}\right)\left(1+L_{-k}\left[\beta_{-k}-1\right]\right)
$$

where $\beta_{-k}$ is the albedo of the surface of segment $-k$. A cyclic trajectory is a series of finite segments $\left\{L_{N-1}, L_{n-2}, \cdots, L_{2}, L_{1}, L_{0}\right\}$, while segments with negative indexes $\left\{L_{-1}, L_{-2}, \cdots, L_{-(N-1)}\right\}$ are associated with intercepted surfaces with a relative weight of $L_{-k}$. For the crossing of a unique surface identified by its index $-k$, a weight of $L_{-k}=1$ is equivalent to applying a desired albedo condition of $\Phi\left(\overrightarrow{r_{k}}, \vec{\Omega}\right)=\Phi\left(\overrightarrow{r_{k+1}}, \vec{\Omega}\right) \beta_{-k}$.

### 9.15.3 Characteristic Direction Probabilities (CDP)

On-going improvements are being elaborated for the method of characteristics. A promising technique is that of Characteristic Direction Probabilities ${ }^{50}$. It consists

[^218]in dividing a given volume into subdomains. For the traditional method of characteristic, directions are considered in the whole volume and angular integration is carried out using a quadrature. For CDP, only the cells of a subdomain that are crossed by a given direction are coupled (unlike collision probabilities $P_{i j}$ for instance). The lengths of the crossed segments are determined as in the Monte Carlo method. The calculation of the CDP does not require an angular integration and ray tracing is carried out only for each subdomain. The subdomains are then coupled only through the angular flux on the common interfaces of the subdomains. Thus, this method requires less computational time, especially for the ray tracing part, compared to the traditional MOC or $P_{i j}$ methods.

We conclude on this paragraph by pointing out that the advantage of the MOC method is that media can be discretized without the constraint of doing so along preferential directions which would simplify the transport operator. Geometries with complex boundaries can be treated as shown by Fig. 9.16. The windmill mesh of the rodded (boro-silicate) $P W R$ assembly optimizes the flux calculation in regions with moderator by limiting the number of computational cells. A cylindrical mesh would be inefficient wrt the flux precision in these regions. Besides, it should be noted that three rows of fuel cells are added to simulate the environment effect (Fig. 9.17).


Fig. 9.16 Windmill mesh of the rodded (boron silicate) $P W R$ assembly (infography Denis Kerdraon)

Fig. 9.17 Zoom on an elementary pattern of the assembly on the left


### 9.16 Even-Odd Formulation of the Transport Equation

## (Advances Nuclear Science and Technology, vol. 13, p. 155, 1982; Planchard 1995,

 p. 386; Stacey 2001, p. 503).The even-odd formulation of the transport equation involves calculating the flux to the minimization of a quadratic functional for which the stationary point is sought. ${ }^{51}$ This method has been described in several US works and was introduced in France by Daniel Verwaerde ${ }^{52}$ from CEA as from 1985.

[^219]It is interesting as it divides the phase space into two, thereby explaining the running speed, especially for isotropic cases.

### 9.16.1 Even-Odd Flux Equation

Starting from the time-independent integro-differential form of the transport equation with isotropic sources and isotropic scattering ${ }^{53}$ :

$$
\begin{aligned}
\vec{\Omega} & \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E, \vec{\Omega})+\Sigma_{t}(\vec{r}, E) \quad \Phi(\vec{r}, E, \vec{\Omega}) \\
& =S(\vec{r}, E)+\int_{0}^{\infty} d E^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime} \rightarrow E\right) \int_{4 \pi} d \vec{\Omega}^{\prime} \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
\end{aligned}
$$

For the multi-group approximation with isotropic scattering hypothesis, the equation for an energy group $g$ is written as:
project after France decided to stop nuclear tests in the Pacific Ocean. This programme became more and more important as it was on that Laser MegaJoule project and him that the "deterrent" nature was conceived. Between 2000 and 2004, he became the director of the CEA center at Bruyères-le-Châtel where he was in charge of the Ter@tec, which is a pole of European knowhow for high performance computing which deals with intensive calculations for industries. Since April 2007, he is in charge of the Direction of Military Applications of the CEA.


[^220]\[

$$
\begin{aligned}
& \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{g}(\vec{r}, \vec{\Omega})+\Sigma_{t g}(\vec{r}) \Phi_{g}(\vec{r}, \vec{\Omega}) \\
& \quad=S_{g}(\vec{r})+\Sigma_{s g}(\vec{r}) \int_{4 \pi} d \vec{\Omega}^{\prime} \Phi_{g}\left(\vec{r}, \vec{\Omega}^{\prime}\right)=S_{g}(\vec{r})+\Sigma_{s g}(\vec{r}) \Phi_{g}(\vec{r})
\end{aligned}
$$
\]

Afterwards, to simplify the notations, the index $g$ is not written in the equations. The angular flux may be expressed as the sum of two components called the even parity flux and the odd flux. The even-odd equation is expressed as:

$$
\Phi(\vec{r}, \vec{\Omega})=\Phi^{+}(\vec{r}, \vec{\Omega})+\Phi^{-}(\vec{r}, \vec{\Omega})
$$

with:

$$
\left\{\begin{array}{l}
\Phi^{+}(\vec{r}, \vec{\Omega})=\frac{1}{2}[\Phi(\vec{r}, \vec{\Omega})+\Phi(\vec{r},-\vec{\Omega})] \text { the even flux being } \Phi^{+}(\vec{r}, \vec{\Omega})=\Phi^{+}(\vec{r},-\vec{\Omega}) \\
\Phi^{-}(\vec{r}, \vec{\Omega})=\frac{1}{2}[\Phi(\vec{r}, \vec{\Omega})-\Phi(\vec{r},-\vec{\Omega})] \text { the odd flux being } \Phi^{-}(\vec{r}, \vec{\Omega})=-\Phi^{-}(\vec{r},-\vec{\Omega})
\end{array}\right.
$$

It should be noted that:

$$
\begin{aligned}
\int_{\Omega} \Phi^{-}(\vec{r}, \vec{\Omega}) d \vec{\Omega} & =\int_{\Omega} \frac{1}{2}[\Phi(\vec{r}, \vec{\Omega})-\Phi(\vec{r},-\vec{\Omega})] d \Omega \\
& =\frac{1}{2}\left[\int_{-2 \pi}^{2 \pi} \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}-\int_{-2 \pi}^{2 \pi} \Phi(\vec{r},-\vec{\Omega}) d \vec{\Omega}\right]=0
\end{aligned}
$$

since the following change of variable is:

$$
\int_{-2 \pi}^{2 \pi} \Phi(\vec{r},-\vec{\Omega}) d \vec{\Omega}=-\int_{2 \pi}^{-2 \pi} \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}=\int_{-2 \pi}^{2 \pi} \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}
$$

The angularly-integrated scalar flux corresponds to the angular integral of the even flux:

$$
\Phi(\vec{r})=\int_{\Omega} \Phi^{+}(\vec{r}, \vec{\Omega}) d \vec{\Omega}
$$

The neutron current is given by:

$$
\vec{J}(\vec{r})=\int_{\Omega} \Phi(\vec{r}, \vec{\Omega}) \vec{\Omega} d \vec{\Omega}=\int_{\Omega} \Phi^{-}(\vec{r}, \vec{\Omega}) \vec{\Omega} d \vec{\Omega}+\underbrace{\int_{\Omega} \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} d \vec{\Omega}}_{\overrightarrow{0} \text { since } \Phi^{+} \text {even }}=\int_{\Omega} \Phi^{-}(\vec{r}, \vec{\Omega}) \vec{\Omega} d \vec{\Omega}
$$

The diffusion equation for angle $-\vec{\Omega}$ is expressed as:

$$
-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r},-\vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r},-\vec{\Omega})=S(\vec{r})+\Sigma_{s}(\vec{r}) \Phi(\vec{r})
$$

Subtracting this equation from the diffusion equation expressed in $\vec{\Omega}$, the scattering term and the source which do not depend on the angle can be cancelled:

$$
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r},-\vec{\Omega})+\Sigma_{t}(\vec{r})(\Phi(\vec{r}, \vec{\Omega})-\Phi(\vec{r},-\vec{\Omega}))=0
$$

i.e. using the definition of the even flux:

$$
\begin{array}{ll} 
& \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi^{-}(\vec{r}, \vec{\Omega})=0 \\
\text { or even: } & \Phi^{-}(\vec{r}, \vec{\Omega})=-\frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})
\end{array}
$$

The diffusion equation can then be written using only the even component of the flux and the scalar flux, thereby leading to an elliptic formulation of the problem, sometimes called the Feautrier formulation ${ }^{54}$ :
$-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}}\left[\frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})\right]+\Sigma_{t}(\vec{r}) \Phi^{+}(\vec{r}, \vec{\Omega})=S(\vec{r})+\Sigma_{s}(\vec{r}) \Phi(\vec{r})$
which may be expressed as:
Even flux diffusion equation :

$$
\begin{align*}
& -\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}}\left[\frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})\right] \\
& \quad+\frac{\Sigma_{s}(\vec{r})}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})+\left(\Sigma_{t}(\vec{r})-\Sigma_{s}(\vec{r})\right) \Phi^{+}(\vec{r}, \vec{\Omega})=S \tag{9.42}
\end{align*}
$$

The solution to this second-order equation leads to the even flux. The neutron current can also be defined in terms of the even flux only:

[^221]Fig. 9.18 Reflective condition of the angular flux


$$
\vec{J}(\vec{r})=\int_{\Omega} \vec{\Omega} \frac{1}{\Sigma_{t}(\vec{r})} \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega}) \cdot \vec{\Omega} d \vec{\Omega}
$$

It can be noted that knowing the even flux leads to the scalar flux and the current simply by angular integration. As for the boundary conditions, if the angular flux has a reflective condition (Fig. 9.18):

$$
\Phi(\vec{r}, \vec{\Omega})=\Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right)
$$

then, the even flux has the same property:

$$
\Phi^{+}(\vec{r}, \vec{\Omega})=\Phi^{+}\left(\vec{r}, \vec{\Omega}^{\prime}\right)
$$

The void condition around the domain of boundary $\Gamma$ is expressed in scalar flux as:

$$
\Phi(\vec{r}, \vec{\Omega})=0 \quad \text { for } \quad \vec{r} \in \Gamma \quad \text { and } \quad \vec{\Omega} . \vec{n}<0
$$

and the even flux for outgoing directions from the domain:

$$
-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \quad \Phi^{+}(\vec{r}, \vec{\Omega})=0 \quad \text { for } \quad \vec{r} \in \Gamma \quad \text { and } \quad \vec{\Omega} \cdot \vec{n}>0
$$

and for incoming directions of the domain:
Void boundary conditions in terms of the even flux:

$$
\begin{equation*}
-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})-\Sigma_{t}(\vec{r}) \quad \Phi^{+}(\vec{r}, \vec{\Omega})=0 \quad \text { for } \vec{r} \in \Gamma \text { and } \vec{\Omega} \cdot \vec{n}<0 \tag{9.43}
\end{equation*}
$$

The even flux formulation has the advantage of requiring the resolution of the equation on the half space of $2 \pi$ solid angle due to parity considerations, since the even flux is identical in the "mirror" half-space. Compared to the usual integrodifferential equation which necessitates the calculation of the solution for all the directions $\vec{\Omega}$, the even flux formulation requires half of the unknowns for the same precision. ${ }^{55}$ However, the isotropic scattering hypothesis simplifies the equation

[^222]considerably and the use of anisotropy (due to water for instance) reduces the advantage of the even-odd formulation and thus, the computation of the solution becomes much more complex, or even useless compared to the usual approach. It should also be noted that the fact that there is the inverse of the total cross section renders the use of this formulation complicated for neutron transport in vacuum. Furthermore, this approach corresponds to the fact that the operator from Eq. (9.42) is a self-adjoint elliptic operator (symmetrical) for which the inverse is positive, and thus the variational approach through the minimization of a functional is applicable, with the use of several numerical methods such as finite elements ${ }^{56}$ in the 1980 's. The principles of the variational approach will be developed without nevertheless, describing thoroughly the numerical methods that can be found in specific textbooks such as (Lewis and Miller 1993).

### 9.16.2 Variational Nodal Method of the Even-Odd Formulation

In $1961,{ }^{57}$ V. S. Vladimirov ${ }^{58}$ introduced the following functional:

[^223]
(USSR Academy of Science, photograph unknown)

Even flux functional:

$$
\begin{align*}
F\left[\Phi^{+}\right]= & \int d r^{3} \int d \vec{\Omega}\left[\frac{1}{\Sigma_{t}(\vec{r})}\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}-\Sigma_{t}(\vec{r})\left[\Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}-\Sigma_{s}(\vec{r}) \Phi^{2}(\vec{r})-2 \Phi(\vec{r}) S(\vec{r})\right] \\
& +\int_{\Gamma} d \Gamma \int d \vec{\Omega}|\vec{n} \cdot \vec{\Omega}| \Phi^{+2}(\vec{r}, \vec{\Omega}) \tag{9.44}
\end{align*}
$$

It can be proved that Eq. (9.42) is the Euler-Lagrange equation of that functional. It will be differentiated by introducing a perturbation of the even flux and the scalar flux as:

$$
\begin{gathered}
\left\{\begin{array}{c}
\Phi^{+}(\vec{r}, \vec{\Omega})=\Phi_{0}^{+}(\vec{r}, \vec{\Omega})+\delta \Phi^{+}(\vec{r}, \vec{\Omega}) \\
\Phi(\vec{r})=\Phi_{0}(\vec{r})+\delta \Phi(\vec{r})
\end{array}\right. \\
\left\{\begin{array}{c}
F\left[\Phi^{+}\right]=F\left[\Phi_{0}^{+}\right]+ \\
2 \int d r^{3} \int d \vec{\Omega}\left[\frac{1}{\Sigma_{t}(\vec{r})}\left[\vec{\Omega} \cdot \overrightarrow{g r a d} \delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right]\right. \\
\left.+\Sigma_{t}(\vec{r}) \Phi_{0}^{+}(\vec{r} \vec{\Omega}) \delta \Phi^{+}(\vec{r} \vec{\Omega})-\left[\Sigma_{s}(\vec{r}) \Phi(\vec{r})+S(\vec{r})\right] \delta \Phi(\vec{r})\right] \\
+\int_{\Gamma} d r^{3} \int d \vec{\Omega}\left[\frac { 1 } { \Sigma _ { t } ( \vec { r } ) } \left[\vec{\Omega} \cdot \overrightarrow{\left.\left.\operatorname{grad} \delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}+\Sigma_{t}(\vec{r})\left[\delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}-\Sigma_{s}(\vec{r})[\delta \Phi(\vec{r})]^{2}\right]}\right.\right. \\
+2 \int_{\Gamma} d \Gamma \int d \vec{\Omega} \vec{n} \cdot \vec{\Omega} \Phi_{0}^{+}(\vec{r}, \vec{\Omega}) \delta \Phi^{+}(\vec{r}, \vec{\Omega})+\int_{\Gamma} d \Gamma \int d \vec{\Omega} \cdot|\vec{n} \cdot \vec{\Omega}|\left[\delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}
\end{array}\right.
\end{gathered}
$$

From a symbolic point of view, the terms in $\delta \Phi^{+}(\vec{r}, \vec{\Omega})$ and $\delta \Phi(\vec{r})$ can be grouped together, just as $\left[\delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}$ and $[\delta \Phi(\vec{r})]^{2}$, thereby ending with the following expression:

$$
F\left[\Phi^{+}\right]=F\left[\Phi_{0}^{+}\right]+\delta F+\delta^{2} F
$$

The first-order differential term $\delta F$ is then written as:

$$
\begin{aligned}
& 2 \int d r^{3} \int d \vec{\Omega}\left[\frac{1}{\Sigma_{t}(\vec{r})}\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right]\right. \\
& \left.+\Sigma_{t}(\vec{r}) \Phi_{0}^{+}(\vec{r}, \vec{\Omega}) \delta \Phi^{+}(\vec{r}, \vec{\Omega})-\left[\Sigma_{s}(\vec{r}) \Phi_{0}(\vec{r})+S(\vec{r})\right] \delta \Phi(\vec{r})\right] \\
& +2 \int_{\Gamma} d \Gamma \int d \vec{\Omega}|\vec{n} \cdot \vec{\Omega}| \Phi_{0}^{+}(\vec{r}, \vec{\Omega}) \delta \Phi^{+}(\vec{r}, \vec{\Omega})
\end{aligned}
$$

Using:

$$
\overrightarrow{\operatorname{grad}}(f g)=f \overrightarrow{g r a d} g+g \overrightarrow{g r a d} f
$$

The product of gradients in the integral kernel is substituted by:

$$
\begin{aligned}
& \frac{1}{\Sigma_{t}(\vec{r})} {\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi^{+}(\vec{r}, \vec{\Omega})\right]\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right] } \\
& \quad=\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}}\left[\frac{1}{\Sigma_{t}(\vec{r})} \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right] \\
&-\delta \Phi^{+}(\vec{r}, \vec{\Omega}) \cdot \vec{\Omega} \cdot \frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})
\end{aligned}
$$

and, given that:

$$
\begin{aligned}
\vec{\Omega} & . \overrightarrow{\operatorname{grad}}\left[\frac{1}{\Sigma_{t}(\vec{r})} \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right] \\
& =\operatorname{div} \vec{\Omega} \cdot\left[\frac{1}{\Sigma_{t}(\vec{r})} \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right]
\end{aligned}
$$

along with the application of the Ostrogradski theorem to transform a volume integral into a surface integral, the following equation is reached:

$$
\begin{aligned}
& \int d r^{3} \int d \vec{\Omega} d i v \vec{\Omega} \cdot\left[\frac{1}{\Sigma_{t}(\vec{r})} \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right] \\
& \quad=\int_{\Gamma} d \Gamma \int d \vec{\Omega} \vec{n} \cdot \vec{\Omega}\left[\frac{1}{\Sigma_{t}(\vec{r})} \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right]
\end{aligned}
$$

Since the perturbation of the scalar flux is a consequence of the increment of the even flux:

$$
\Phi(\vec{r})=\Phi_{0}(\vec{r})+\delta \Phi(\vec{r})=\Phi_{0}(\vec{r})+\int d \vec{\Omega} \delta \Phi^{+}(\vec{r}, \vec{\Omega})
$$

the increment of the functional can be expressed as:
First-order increment of the even flux functional:

$$
\left\{\begin{array}{l}
\delta F=2 \int d r^{3} \int d \vec{\Omega}\left[-\vec{\Omega} \cdot \frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi_{0}^{+}(\vec{r}, \vec{\Omega})-\left[\Sigma_{s}(\vec{r}) \Phi_{0}(\vec{r})+S(\vec{r})\right]\right] \delta \Phi^{+}(\vec{r}, \vec{\Omega})  \tag{9.45}\\
+2 \int_{\Gamma} d \Gamma \int d \vec{\Omega}\left[|\vec{n} \cdot \vec{\Omega}| \Phi_{0}^{+}(\vec{r}, \vec{\Omega})+\vec{n} \cdot \vec{\Omega} \frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right] \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \\
+2 \int_{\Gamma} d \Gamma \int d \vec{\Omega} \vec{n} \cdot \vec{\Omega}\left[\frac{1}{\Sigma_{t}(\vec{r})} \delta \Phi^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})\right] \delta \Phi^{+}(\vec{r}, \vec{\Omega})
\end{array}\right.
$$

This functional is stationary wrt the even flux variations if the three increment terms are zero. The volume term leads to the even flux equation, thereby justifying the Vladimirov functional a posteriori:
$-\vec{\Omega} \cdot \frac{1}{\Sigma_{t}(\vec{r})} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \quad \Phi_{0}^{+}(\vec{r}, \vec{\Omega})=\Sigma_{s}(\vec{r}) \Phi_{0}(\vec{r})+S(\vec{r})$
Cancelling the second term induces the void boundary condition of Eq. (9.43):

$$
|\vec{n} \cdot \vec{\Omega}| \Sigma_{t}(\vec{r}) \Phi_{0}^{+}(\vec{r}, \vec{\Omega})+\vec{n} \cdot \vec{\Omega} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega})=0
$$

while cancelling the third term results in:

$$
\overrightarrow{\operatorname{grad}} \Phi_{0}^{+}(\vec{r}, \vec{\Omega}) \vec{\Omega}=0 \text { on the boundary } \Gamma
$$

This condition has no particular meaning except in plane geometry where it implies that the even flux is flat at the interface. This is why the third term is forced to zero by rather imposing:

$$
\int d \vec{\Omega} \delta \Phi^{+}(\vec{r}, \vec{\Omega})=\delta \Phi(\vec{r})=0
$$

It means that the flux in the functional must satisfy the conditions imposed at the surface. The numerical consequence is to choose a decomposition of the scalar flux that satisfies the boundary conditions via the basis functions for the flux expansion. Hence, if the even flux satisfies the condition that the first order expansion of the Vladimirov expansion is zero, i.e. the functional is stationary, then that flux verifies the even flux equation and its associated boundary conditions. A similar functional may be generated for other boundary conditions (albedo, surface sources, etc.). The analysis of the second-order term $\delta^{2} F$ shows that the latter is positive, thereby accounting for the fact that the minimum is sought at $\Phi_{0}^{+}$.

### 9.16.3 Ritz Method

(Marchuk and Agochkov 1985, p. 25; Reddy 1984, p. 37; Strang and Fix 1973, p. 24).

One way of treating the functional is to use the Ritz method. The even flux is expanded on the basis of orthogonal even functions for space and angle:

$$
\Phi^{+}(\vec{r}, \vec{\Omega})=\sum_{i} \varphi_{i}^{+} f_{i}(\vec{r}, \vec{\Omega})
$$

For the space variable, the Legendre polynomials $P_{n}(x)$ are employed as orthogonal functions, while in angle, the spherical harmonic functions are introduced. The Legendre polynomials are calculated using the Rodrigues formula:

$$
\begin{equation*}
\text { Rodrigues formula: } \quad P_{n}(x)=\frac{1}{2^{n} n!} \frac{d^{n}}{d x^{n}}\left(x^{2}-1\right)^{n} \tag{9.46}
\end{equation*}
$$

The spherical harmonics $Y_{n}^{m}(\theta, \varphi)$ are the eigenfunctions of the Laplace operator in spherical coordinates and are expressed using the associated Legendre functions, derived from the Legendre polynomials as follows:

$$
\begin{equation*}
\text { Associated Legendre functions: } \left.\quad P_{n}^{m}(x)=(-1)^{m} \sqrt{\left(1-x^{2}\right)}\right)^{m} \frac{d^{m}}{d x^{m}} P_{n}(x) \tag{9.47}
\end{equation*}
$$

The spherical harmonics are normalized to 1 are given by:
Spherical harmonics: $\quad Y_{n}^{m}(\theta, \varphi)$

$$
\begin{equation*}
=(-1)^{m} \sqrt{\frac{(2 n+1)(n-m)!}{4 \pi(n+m)!}} P_{n}^{m}(\cos \theta) e^{i \varphi m} \tag{9.48}
\end{equation*}
$$

In matrix form, the following is obtained:

$$
\left\{\begin{array}{c}
\varphi^{+}=\left(\begin{array}{c}
\varphi_{1}^{+} \\
\varphi_{2}^{+} \\
\vdots \\
\varphi_{n}^{+}
\end{array}\right) \\
f(\vec{r}, \vec{\Omega})=\left(\begin{array}{c}
f_{1}(\vec{r}, \vec{\Omega}) \\
f_{2}(\vec{r}, \vec{\Omega}) \\
\vdots \\
f_{n}(\vec{r}, \vec{\Omega})
\end{array}\right) f^{T}(\vec{r}, \vec{\Omega})=\left(\varphi_{1}^{+}, \varphi_{2}^{+}, \ldots, \varphi_{n}^{+}\right)
\end{array}\right.
$$

hence, the matrix form of the even flux is:

$$
\Phi^{+}(\vec{r}, \vec{\Omega})=\varphi^{+T} f(\vec{r}, \vec{\Omega})=f^{T}(\vec{r}, \vec{\Omega}) \varphi^{+}
$$

With this notation:

$$
\left[\Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}=\left(\varphi^{+T} f(\vec{r}, \vec{\Omega})\right)\left(f^{T}(\vec{r}, \vec{\Omega}) \varphi^{+}\right)=\varphi^{+T}\left(f(\vec{r}, \vec{\Omega}) f^{T}(\vec{r}, \vec{\Omega})\right) \varphi^{+}
$$

and:

$$
\begin{aligned}
& {\left[\Phi(\vec{r}]^{2}=\int d \vec{\Omega} \Phi^{+}(\vec{r}, \vec{\Omega}) \int d \vec{\Omega}^{\prime} \Phi^{+}\left(\vec{r}, \vec{\Omega}^{\prime}\right)\right.} \\
& \quad=\int d \vec{\Omega}\left(\varphi^{+T} f(\vec{r}, \vec{\Omega})\right) \int d \vec{\Omega}^{\prime}\left(f^{T}\left(\vec{r}, \vec{\Omega}^{\prime}\right) \varphi^{+}\right) \\
& =\varphi^{+T}\left(\int d \vec{\Omega} f(\vec{r}, \vec{\Omega}) \int d \vec{\Omega}^{\prime} f^{T}\left(\vec{r}, \vec{\Omega}^{\prime}\right)\right) \varphi^{+}
\end{aligned}
$$

Introducing these expressions in the functional leads to a matrix equation known as a reduced functional:

$$
F[\varphi]=\varphi^{+T} \mathrm{~A} \varphi^{+}-2 \varphi^{+T} \mathrm{~S}
$$

where $A$ is a square symmetric matrix and $S$ is the source column vector:

With a perturbation $\delta \varphi^{+}$of the even flux vector such that:

$$
\varphi^{+}=\varphi_{0}^{+}+\delta \varphi^{+}
$$

the reduced functional is written by noting that $\mathrm{A}^{T}=\mathrm{A}$ :

$$
F\left[\varphi^{+}\right]=\underbrace{\varphi_{0}^{+T} \mathrm{~A} \varphi_{0}^{+}-2 \varphi_{0}^{+T} \mathrm{~S}}_{F\left[\varphi_{0}^{+}\right]}+\underbrace{2 \delta \varphi^{+T}\left(\mathrm{~A} \varphi_{0}^{+}-\mathrm{S}\right)}_{\delta F\left[\varphi_{0}^{+}\right]}+\underbrace{\delta \varphi^{+T} \mathrm{~A} \delta \varphi^{+}}_{\delta^{2} F\left[\varphi_{0}^{+}\right]}
$$

Minimizing that functional can be carried out by cancelling the first-order term $\delta F\left[\varphi_{0}^{+}\right]$, i.e. by solving the linear system:

$$
\mathrm{A} \varphi_{0}^{+}=\mathrm{S}
$$

Therefore, if the flux $\Phi^{+}(\vec{r}, \vec{\Omega})$ is not known, it can be approximated by a series of even functions for which the coefficients are the solutions to the linear system. In practice, it can be noted that other functional may be used, especially:

$$
\begin{aligned}
& F\left[\Phi^{+}\right]=\int d^{3} r \int d \vec{\Omega}\left[\frac{1}{\Sigma_{t}(\vec{r})}\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}-\Sigma_{t}(\vec{r})\left[\Phi^{+}(\vec{r}, \vec{\Omega})\right]^{2}-\Sigma_{s}(\vec{r}) \Phi^{2}(\vec{r})-2 \Phi(\vec{r}) S(\vec{r})\right] \\
& +2 \int_{\Gamma} d \Gamma d \vec{\Omega}|\vec{n} \cdot \vec{\Omega}| \Phi^{+}(\vec{r}, \vec{\Omega})
\end{aligned}
$$

which differs from Eq. (9.44) only by the surface term where the even flux is not squared and the surface term is doubled. A nodal functional is created by discretizing space into regions of volume $V_{i}$ with interfaces $\Gamma_{m}$, and using the odd flux at the crossing of each interface as the Lagrange multiplier [for the theory on Lagrange multipliers in minimization, refer to (Bertsekas 1982)]:

$$
\begin{aligned}
& F\left[\Phi^{+}, \Phi^{-}\right]=\sum_{i} V_{i} \int d \vec{\Omega}\left[\frac{1}{\Sigma_{t i}}\left[\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{i}^{+}\right]^{2}-\sum_{t i} \Phi_{i}^{+2}-\Sigma_{s i} \Phi_{i}^{2}-2 \Phi_{i}^{2} S_{i}\right] \\
& \quad+2 \sum_{m} \int_{\Gamma_{m}} d \Gamma \int d \vec{\Omega} \vec{n} \cdot \vec{\Omega}\left(\Phi_{i}^{+}-\Phi_{j}^{+}\right) \Phi_{m}^{-}
\end{aligned}
$$

where $i$ and $j$ are the indices of the mesh cells that touch the interface $m$. Multiplying the odd flux is useful to constraint the neutron balance in each cell. If the cross sections are constant in each mesh cell, the mean neutron balance is guaranteed for any function $\Phi^{+}$, i.e. if $\Phi^{+}=\overline{\Phi^{+}}+\delta \Phi^{+}$with $\int d^{2} r \int d \vec{\Omega} \delta \Phi^{+}=0$ and that the reduced functional is stationary wrt variation in $\overline{\Phi^{+}}$. Then, the corresponding EulerLagrange equation for the minimization of the functional is exactly equal to the neutron balance per cell:

$$
\left(\Sigma_{t i}-\Sigma_{s i}\right) \overline{\Phi^{+}} V_{i}=\int_{\Gamma_{m}} d \Gamma \vec{n} \cdot \overrightarrow{J_{m}}=\int_{V_{i}} S_{i} d^{3} r=\text { sources in the volume }
$$

### 9.17 Variational Method for Time-Dependent Problems

The variational approach can be extended to the time-dependent Boltzmann equation. ${ }^{59}$ Let the time-dependent equation be:

$$
\begin{aligned}
& \frac{1}{v} \frac{\partial \Phi(\vec{r}, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, t)+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega}, t) \\
& \quad-\int_{0}^{\infty} d E^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime}\right) \int_{4 \pi} d \vec{\Omega}^{\prime} \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}, t\right) \\
& \quad=S(\vec{r}, \vec{\Omega}, t)
\end{aligned}
$$

The notations are simplified by removing the time dependence and using the operator:

$$
\Sigma[\Phi(\vec{r}, \vec{\Omega})] \equiv \Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})-\int_{0}^{\infty} d E^{\prime} \Sigma_{S}\left(\vec{r}, E^{\prime}\right) \int_{4 \pi} d \vec{\Omega}^{\prime} \Phi\left(\vec{r}, E^{\prime}, \vec{\Omega}^{\prime}\right)
$$

The boundary conditions of the problem can be of several types:

[^224]\[

\left\{$$
\begin{array}{lll}
\Phi\left(\vec{r}_{s}, \vec{\Omega}, t\right)=\Phi\left(\vec{r}_{s}, \vec{\Omega}, t\right) & \text { at surface } S_{s} \text { for } \vec{\Omega} \cdot \vec{n}<0 \quad \text { (surface with imposed current) } \\
\Phi\left(\vec{r}_{s}, \vec{\Omega}, t\right)=0 \quad \text { at surface } S_{n} \text { for } \vec{\Omega} \cdot \vec{n}<0 \quad \text { (void surface) } \\
\Phi\left(\vec{r}_{s}, \vec{\Omega}, t\right)=\Phi\left(\vec{r}_{s}, \vec{\Omega}^{\vee}, t\right) & \text { at surface } S_{r} \text { for } \vec{\Omega} \cdot \vec{n}=-\vec{\Omega}^{\vee} \cdot \vec{n} \quad \text { (reflecting surface) }
\end{array}
$$\right.
\]

As for the initial condition $\Phi(\vec{r}, \vec{\Omega}, 0)$, a zero value can be always employed by noting that the transport equation is invariant by substituting the flux by a flux increment $\Phi(\vec{r}, \vec{\Omega}, t)-\Phi(\vec{r}, \vec{\Omega}, 0)$, the source by a source increment and the boundary condition $\Phi_{S}\left(\vec{r}_{s}, \vec{\Omega}, t\right)$ by the increment $\Phi_{S}\left(\vec{r}_{s}, \vec{\Omega}, t\right)-\Phi_{S}\left(\vec{r}_{s}, \vec{\Omega}, 0\right)$. Ackroyd and Oliveira proposed the functional $V_{\tau}(\psi)$ applied to the test function $\psi$, obtained by the integration over the time interval $[0, \tau]$ and the reactor volume $V$ :
where $\langle f, g\rangle=\int_{\Omega} f g d \vec{\Omega} \cdot V_{\tau}(\psi)$ is a measure of the precision of the approximation $\psi$ of the exact flux $\Phi$ which is to be minimized. The error $\varepsilon=\Psi-\Phi$ is injected in the functional:

$$
\begin{aligned}
V_{\tau}(\varepsilon) & =V_{\tau}(\psi)-\underbrace{V_{\tau}(\Phi)}_{0} \\
& =\int_{t=0}^{t=\tau} d t\left\{\begin{array}{l}
\int_{V} d^{3} r\left\langle\frac{1}{v} \frac{\partial \varepsilon}{v} \frac{\varepsilon}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \varepsilon+\Sigma[\varepsilon], \Sigma^{-1}\left[\frac{1}{v} \frac{\partial \varepsilon}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \varepsilon+\Sigma[\varepsilon]\right]\right\rangle \\
+2 \int_{S_{n} \cup S_{s}} \int_{\vec{\Omega} \cdot \vec{n}<0}|\vec{\Omega} \cdot \vec{n}| \varepsilon^{2} d \vec{\Omega} d^{2} r_{s}
\end{array}\right\}
\end{aligned}
$$

Instead of minimizing $V_{\tau}(\psi)$, the problem is expressed such as a maximum is sought as it is much easier numerically. Hence, the functional $K_{\tau}(\psi)$ to be maximized is defined as:

$$
K_{\tau}(\psi)+V_{\tau}(\psi)=\int_{t=0}^{t=\tau} d t\left\{\int_{V} d^{3} r\left\langle S, \Sigma^{-1}[S]\right\rangle+2 \int_{S_{s}} \int_{\vec{\Omega} \cdot \vec{n}<0}|\vec{\Omega} \cdot \vec{n}| \Phi_{s}^{2} d \vec{\Omega} d^{2} r_{s}\right\}
$$

i.e.:

$$
\begin{aligned}
& K_{\tau}(\Psi)= \int_{t=0}^{t=\tau} d t\left\{\begin{array}{l}
2 \int_{V} d^{3} r\left(\left\langle\frac{1}{v} \frac{\partial \Psi}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\left.\left.\operatorname{grad} \Psi, \Sigma^{-1}[S]\right\rangle+\langle\Psi, S\rangle\right)}\right.\right. \\
+4 \int_{S_{S}} \int_{\vec{\Omega} \cdot n<0}|\vec{\Omega} \cdot \vec{n}| \Phi_{s}^{2} d \vec{\Omega} d^{2} r_{s} \\
-\int_{V} d^{3} r\left(\left\langle\frac{1}{v} \frac{\partial \Psi}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad} \Psi} \Psi, \Sigma^{-1}\left[\frac{1}{v} \frac{\partial \Psi}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad} \Psi}\right]\right\rangle+\langle\Psi, \Sigma[\Psi]\rangle\right) \\
-2 \int_{S_{n} \cup S_{s}} \int_{\vec{\Omega} \cdot \vec{n}<0}|\vec{\Omega} \cdot \vec{n}| \Psi^{2} d \vec{\Omega} d^{2} r_{s}
\end{array}\right\} \\
& \quad-\frac{1}{v} \int_{V} d^{3} r\langle\Psi(\tau), \Psi(\tau)\rangle
\end{aligned}
$$

### 9.18 Gauss-Seidel Method for Sources in Time-Dependent Problems

The time-dependent multi-group integro-differential equation is written as:

$$
\begin{aligned}
\frac{1}{v_{g}} & \frac{\partial \Phi_{g}(\vec{r}, \vec{\Omega}, t)}{\partial t}+\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{g}(\vec{r}, \vec{\Omega}, t)+\Sigma_{t, g}(\vec{r}) \Phi_{g}(\vec{r}, \vec{\Omega}, t) \\
& =\sum_{g^{\prime}=1}^{G} \int_{4 \pi} d \vec{\Omega}^{\prime} \Sigma_{s}^{g \prime \rightarrow g}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}\right) \Phi_{g^{\prime}}\left(\vec{r}, \vec{\Omega}^{\prime}, t\right)+S_{g}(\vec{r}, \vec{\Omega}, t)
\end{aligned}
$$

and is often treated numerically using the $\theta$-scheme, i.e. the mutigroup flux is substituted by the weighting of the flux over the current time step and that of the previous step:

$$
\Phi_{g}\left(\vec{r}, \vec{\Omega}, t_{n+1}\right)=\theta \Phi_{g}^{n+1}(\vec{r}, \vec{\Omega})+(1-\theta) \Phi_{g}^{n}(\vec{r}, \vec{\Omega})
$$

The scheme is an implicit scheme for $\theta=1$, but stability criteria allow the use of a semi-implicit scheme with $\theta \in[1 / 2,1]$, as in the Crank-Nicholson scheme with $\theta=1 / 2$. The latter is of order 2 in time while for any other value of $\theta$, it is of order 1 . Hence, by omitting the variables $(\vec{r}, \vec{\Omega})$ for concision, the equation to be solved is:

$$
\begin{aligned}
& \frac{1}{v_{g}} \frac{\Phi_{g}^{m+1}}{\theta \Delta t}+\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{g}^{m+1}+\Sigma_{t, g} \Phi_{g}^{m+1} \\
& =\frac{(1-\theta)}{\theta} \sum_{g^{\prime}=1}^{G} \Sigma_{s}^{g \prime \rightarrow g} \Phi_{g^{\prime}}^{m+1}+\sum_{g^{\prime}=1}^{G} \Sigma_{s}^{g \prime \rightarrow g} \Phi_{g^{\prime}}^{m}+S_{g}^{m}+\frac{1}{v_{g}} \frac{\Phi_{g}^{m}}{\theta \Delta t} \\
& \quad-\frac{(1-\theta)}{\theta}\left(\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{g}^{m}+\Sigma_{t, g} \Phi_{g}^{m}\right)
\end{aligned}
$$

The iteration over the sources consists in benefitting of the triangular nature of the slowing-down matrix by calculating the flux for the fast groups, and then substituting the last flux evaluation from the higher-energy groups in the source term of the current group. Hence, for the current group $g$, the equation to solve is:

$$
\begin{aligned}
\frac{1}{v_{g}} \frac{\Phi_{g}^{m+1}}{\theta \Delta t}+\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{g}^{m+1}+\Sigma_{t, g} \Phi_{g}^{m+1}= & \sum_{g^{\prime}=1}^{g} \Sigma_{s}^{g \prime \rightarrow g} \Phi_{g^{\prime}}^{m+1}+\sum_{g^{\prime}=g+1}^{G} \Sigma_{s}^{g \prime \rightarrow g} \Phi_{g^{\prime}}^{m} \\
& +\chi_{g}\left(\sum_{g^{\prime}=1}^{g} \nu \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}^{m+1}+\sum_{g^{\prime}=g+1}^{G} \nu \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}^{m}\right)+\Delta S_{g}(\theta)
\end{aligned}
$$

where $\Delta S_{g}(\theta)$ represents the remaining source contribution when the slowing-down and fission sources are modeled, and it depends only on the current group and $\theta$. It is recalled here that the fast group is indexed by 1 . This technique is called the GaussSeidel iteration for sources, by analogy with the iterative method with the same name for linear systems. This technique is also applicable in diffusion theory.

### 9.19 Probabilistic Approach: The Monte Carlo Method

(Baur 1985, p. 234; Chen et al. 2002; Dautray 1989; Doucet et al. 2001; Dupree and Fraley 2002; Fishman 1995; Gentle 2005; Hoffmann and Schreiber 2002; Lapeyre et al. 1998; Liu 2001; Robert and Casella 2004; Rubinstein 1981; Spanier and Gelbard 1969; Williams 1979).

### 9.19.1 Fundamental Concepts of the Monte Carlo Method

The Monte Carlo originates from the works that led to the atomic bomb during the 1940's. The term is attributed to John von Neumann (1903-1957), whose work on mathematics and information technology is highly prominent, as an idealization of
the use of random numbers as those occurring in a casino. In France, the method has been applied by Jean-Claude Nimal ${ }^{60}$ and Jean Rastoin ${ }^{61}$ as of $1965{ }^{62}$ for neutron transport. Historically, it is known that in 1777, Georges-Louis Leclerc, Count of Buffon, a renowned naturalist (1707-1788) and Superintendant to the Jardin des Plantes (botanical gardens) in Paris, proposed a recreative game whereby a needle of length $\ell$ is thrown randomly on the parquet (wooden flooring) with wooden strips of width $d>\ell$. It can be shown that the probability that the needle intersects the parallel lines of the wooden strips is of $2 \ell /(\pi d)$. This probability is obtained (slowly!) by repeating the needle throws a large number of times and by counting the number of "winning" throws compared to the total. The choice of $d=2 \ell$ leads to an intersecting probability of $1 / \pi$. In general, a problem with a unique solution $Y$ is solved by constructing a statistical process [Markov chain (Iosifescu et al. 2007)] constituted of successive random non-correlated random states called a

[^225]
(Courtesy Rastoin)
${ }^{62}$ Jean-Claude Nimal, Jean Rastoin: Méthodes de Monte-Carlo [Monte Carlo methods], technical report CEA-N 533 (April 1965).
game. A random variable $X$ for the process is called the score and the rule of the game is defined such that the mathematical expectation of $X$ (i.e. the mean from a statistical viewpoint) is equal to $Y$. The game is repeated $n$ independent times to obtain a set $\left\{X_{1}, X_{2}, \ldots, X_{n}\right\}$ with a mean value of:
$$
\overline{X(n)}=\frac{1}{n} \sum_{i=1}^{n} X_{i}
$$

The mathematical expectation ${ }^{63}$ of a quantity $\overline{X(n)}$ is hence equal to $\frac{1}{n} \sum_{i=1}^{n} E\left(X_{i}\right)=\frac{1}{n} \sum_{i=1}^{n} Y=Y$ and by the law of large numbers:

$$
\lim _{n \rightarrow \infty} \overline{X(n)}=E(X(n))=Y
$$

The law of large numbers was established by Bernouilli in the seventeenth century and states that the random variable $\overline{X(n)}$ has a Gaussian distribution of mathematical expectation $Y$ and of variance:

$$
\sigma_{\bar{X}(n)}^{2}=\frac{\sigma_{X}^{2}}{n}=\frac{E\left((X-E(X))^{2}\right)}{n}=\frac{E\left(X^{2}\right)-(E(X))^{2}}{n}
$$

which means that the variance decreases as $1 / \sqrt{n}$, which is very slow. It should also be pointed out that the variance of the mean value is the variance of the variable divided by the number of terms used to compute the mean. The probability $p(\varepsilon)$ such that $\overline{X(n)}$ belongs to the interval between $Y-\varepsilon$ and $Y+\varepsilon$ is given by Lapeyre et al. (1998, p. 5) and Spanier and Gelbard (1969, p. 15):

$$
p(\varepsilon)=\frac{1}{\sqrt{2 \pi} \sigma_{\overline{X(n)}}} \int_{Y-\varepsilon}^{Y+\varepsilon} e^{\frac{(X-Y)^{2}}{2 \sigma^{2}} \overline{\bar{X}(n)}} d X=\operatorname{erf}\left(\frac{\varepsilon}{\sqrt{2} \sigma_{\overline{X(n)}}}\right)
$$

This expression originates from the central limit theorem which states that the sum of independent random variables that are identically distributed, follows a normal distribution, i.e.:

[^226]$$
\lim _{n \rightarrow \infty} P\left(a \leq \frac{X(n)-n E(X)}{\sigma_{\overline{X(n)}} \sqrt{n}} \leq b\right)=\frac{1}{\sqrt{2 \pi}} \int_{a}^{b} e^{-\frac{x^{2}}{2}} d x
$$

For an uncertainty of one standard deviation $\sigma_{\overline{X(n)}}, p\left(\sigma_{\overline{X(n)}}\right)=0.689$; for twice the standard deviation, $p\left(2 \sigma_{\overline{X(n)}}\right)=0.954$; and for three times, $p\left(3 \sigma_{\overline{X(n)}}\right)=0.997$. It should be noted that the central limit theorem does not bound the error but only defines a confidence interval. For the law of large numbers and Gaussian approximation, refer to (Diu et al. 2001, p. 62). The most widespread application of the Monte Carlo method is to calculate the integral of the function $f(x)$ between two bounds $a$ and $b$, given that the function is bounded by $c$ (Fig. 9.19) (Clark and Hansen 1964, p. 254):

A coordinate pair $\left(x_{i}, y_{i}\right)$ is sampled randomly with a random number generator such that $x$ is found between $a$ and $b$, and $y$ is found between 0 and $c$ [if the latter samples numbers between 0 and 1 uniformly as it is often the case, this interval may be reached using a variable change, refer especially to Gentle (2005) and Spanier and Gelbard (1969, p. 36)] and the score is counted as:

$$
\begin{cases}y_{i}>f\left(x_{i}\right) & \Rightarrow \quad \text { Score }_{i}=0 \\ y_{i} \leq f\left(x_{i}\right) & \Rightarrow \quad \operatorname{Score}_{i}=1\end{cases}
$$

In this case:

$$
\frac{\int_{a}^{b} f(x) d x}{c(b-a)}=\lim _{n \rightarrow \infty}\left(\frac{1}{n} \sum_{i=1}^{n} \operatorname{Score}_{i}\right)
$$

This technique also allows the calculation of multidimensional integrals (volume integral for instance) without increasing the computational times owing to the higher dimensions. The evaluation of the confidence interval of the calculation

Fig. 9.19 Simple integral calculation by the Monte Carlo method

can be carried out using a non-biased estimator for the variance. Let $\overline{I_{n}}=c(b-a)$ $\frac{1}{n} \sum_{i=1}^{n} \operatorname{Score}_{i}=\frac{1}{n} \sum_{i=1}^{n} X_{i}$ where $X_{i}$ is the non-normalized score obtained from the random number sampling, defined as the empirical sample variance (Lapeyre et al. 1998, p. 6):

$$
V \equiv \frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\overline{I_{n}}\right)^{2}=\frac{n}{n-1} \overline{X_{i}^{2}}-\frac{n}{n-1}\left(\overline{I_{n}}\right)^{2}
$$

$V$ is a non-biased estimator of variance $\sigma^{2}$. In this particular example where the score is equal to 1 or 0 , it should be pointed out that $\overline{\text { Score }_{i}^{2}}=\overline{\text { Score }_{i}}$, i.e. $\overline{X_{i}^{2}}$ $=c(b-a) \overline{X_{i}}$ for the non-normalized score, meaning that if $\lim _{n \rightarrow+\infty} \overline{I_{n}}=I$, then $\lim _{n \rightarrow+\infty} V=I(c(b-a)-I)$. An approached $95 \%$ confidence interval (equal to two standard deviations) is obtained by setting $\bar{\sigma}=\sqrt{V}$ and by replacing $\sigma$ by $\bar{\sigma}$ in the confidence interval given by the central limit theorem. The confidence interval is then equal to $\left[\overline{I_{n}}-2 \bar{\sigma} / \sqrt{n}, \overline{I_{n}}+2 \bar{\sigma} / \sqrt{n}\right]$. The standard deviation on the integral value can also be obtained by setting up a random process for the calculation of the integral value, e.g. by recalculating the integral $L$ successive times $\left(I_{l=1, L}\right)$ by sampling $n$ independent scores: these are cycles of particles. Then, the standard deviation is evaluated using the biased estimator by summing over the square of the discrepancies, averaged by the number of evaluations $L$ :

$$
\sigma_{I}^{2}=E\left((I-E(I))^{2}\right)=\sum_{l=1}^{L} \frac{\left(I_{l}-\bar{I}_{l}\right)^{2}}{L}
$$

Given that the function $f(x)$ is simple to determine, a second and more efficient computation strategy of the mean value is through:

$$
\bar{f}=\frac{1}{n} \sum_{i=1}^{n} f\left(x_{i}\right)
$$

where $x_{i}$ is a random variable sampled uniformly from $[a, b]$ and then calculating the integral value using the mean, as such:

$$
\int_{a}^{b} f(x) d x=(b-a) \bar{f}
$$

The standard deviation is then given by:

$$
\sigma=\sqrt{\frac{\overline{f^{2}}-\bar{f}^{2}}{n}} \text { with } \overline{f^{2}}=\frac{1}{n} \sum_{i=1}^{n}\left[(b-a) f\left(x_{i}\right)\right]^{2}=\frac{(b-a)^{2}}{n} \sum_{i=1}^{n}\left[f\left(x_{i}\right)\right]^{2}
$$

### 9.19.2 Application to Neutron Transport: A Simple 2D Case

(Cashwell and Everett 1959; Hébert 2009, p. 178; Spanier and Gelbard 1969; Goertzel and Kalos, in Progress in nuclear energy, vol. 2, p. 315, 1955; Shultis and Faw 2000, p. 408).

The first applications of the Monte Carlo method to neutron transport are attributed to John von Neumann and Stanley Ulam in the Manhattan Project during the World War II. In the transport chapter, it was pointed out that the collision density can be decomposed as a uncollided flux term $\Sigma_{t} \Phi_{0}(\vec{r}, E, \vec{\Omega})$, then the rate of the first collision flux $\Sigma_{t} \Phi_{1}(\vec{r}, E, \vec{\Omega})$, second collision, etc. This decomposition is called a Von Neumann series:

$$
\Sigma_{t} \Phi(\vec{r}, E, \vec{\Omega})=\sum_{n=0}^{\infty} \Sigma_{t} \Phi_{n}(\vec{r}, E, \vec{\Omega})
$$

Each term of this series can be obtained from the previous one by recurrence using the Peierls collision operator:

$$
\Sigma_{t} \Phi_{n+1}(\vec{r}, E, \vec{\Omega})=\int_{V} K\left[\Sigma_{t} \Phi_{n}\right]
$$

Starting from a source, a Markov chain is set up by assuming that the current event does not depend on the previous one (the neutron "forgets" the means which brought it to its current position in the phase space $(\vec{r}, E, \vec{\Omega})$, thus allowing the use of the Monte Carlo method). The advantage of the Monte Carlo method resides in the fact the Boltzmann equation is not required for simulation purposes Only the physical phenomena such as scattering or absorption are necessary to model the behavior of the neutron population. The neutron furthermore loses track of its history at each collision, thereby implying that its behavior is independent of the previous collisions. Some authors use the term analogue simulation to qualify this approach which is close to the true physical phenomena, ${ }^{64}$ while a non-analogue simulation is carried out by the calculation of integrals. A second advantage of the method comes from the fact that the neutron paths are independent of one another,

[^227]thereby allowing the use of parallel calculators. In the 1990's, the development of multiprocessor computers along with massively parallel clusters has been very beneficial to the Monte Carlo method. Finally, it must be pointed out that geometries may be modeled exactly without any additional cost owing to meshes as with deterministic methods for which computational times are proportional to at least the number of mesh cells. Similarly, as far as the energy variable is concerned, the Monte Carlo method allows the use of pointwise energy cross sections without any multi-group concern. The use of the method will next be illustrated through a simple example: the scattering of neutrons emitted by an isotropic source in a $2 D$ geometry containing a scattering and absorbing material. The problem is simplified by assuming that the medium is a homogeneous mixture of $n$ isotopes for which the neutronic properties such as $\Sigma_{s}^{i}(E), \Sigma_{t}^{i}(E)$ and $\xi_{i}$ are known (Fig. 9.20).

The first question consists in determining the direction and energy of the emitted neutron. Since the source is isotropic, the neutron has an angular emission probability of $1 /(4 \pi)$ and the values of the polar and azimuthal angles $\theta$ (co-latitude) and $\varphi$ (longitude) of the emission are obtained by random sampling in the $[0, \pi]$ interval for $\theta$ and $[0,2 \pi]$ for $\varphi$.

The calculation of the emission angle $\tilde{\theta}$ which corresponds to the projection of the $3 D$ emission direction in the plane $0 x y$ is obtained by projection of the vector $\vec{\Omega}$. The trigonometric formulae lead to the calculation of the sines and cosines of that angle (Fig. 9.21):

$$
\left\{\begin{array}{l}
\sin \widetilde{\theta}=\frac{\sin \theta \cos \varphi}{\sqrt{\cos ^{2} \theta+\sin ^{2} \theta \cos ^{2} \varphi}} \\
\cos \tilde{\theta}=\frac{\cos \theta}{\sqrt{\cos ^{2} \theta+\sin ^{2} \theta \cos ^{2} \varphi}}
\end{array}\right.
$$

It should be noted that it would be wrong to draw angle $\tilde{\theta}$ from the $[0,2 \pi]$ interval considering that neutrons travel only in the $0 x y$ plane as it would lead to a biased simulation. The $2 D$ nature of the geometry does not imply that the neutrons do not move in the third direction. Only the neutron density depends just on $x$ and $y$. The emitted neutron energy is evaluated by recalling the fact that the distribution of neutrons emitted by fission is obtained empirically via the Watt spectrum. The latter

Fig. 9.20 Random neutron path in matter (projection in the plane, referential given by angle $\widetilde{\theta}$ )


Fig. 9.21 Emission angles

is not a uniform law and is given by $\chi(E)=C e^{-a E} \operatorname{sh} \sqrt{b E}$, and for which the constant $C$ is chosen such that $\int_{0}^{20 \mathrm{MeV}} \chi(E) d E=1$. The neutron concentration must all be satisfied with more neutrons being available at 2 MeV . Hence, a random number $x_{0}$ is also sampled from the $[0,1]$ interval so as to calculate the emission energy $E_{0}$ such that:

$$
\int_{0}^{E_{0}} \chi(E) d E=x_{0}
$$

The following collision position is obtained (Spanier and Gelbard 1969, p. 66), by considering that the probability that a neutron travels a distance $\ell$ without any collision is $Q(\ell)=e^{-\Sigma_{t} \ell}$. The first collision probability along path $d \ell$ is expressed as $P(\ell) d \ell=\Sigma_{t} d \ell e^{-\Sigma_{t} \ell}$, which when integrated between 0 and infinity gives 1 . In practice, infinity cannot be used for sampling random numbers. The path of the neutron is thus limited, e.g. to ten times the mean free transport path (i.e. $\ell_{\max }=10$ / $\Sigma_{t}$, it can be widely accepted that the neutron will be absorbed over this path), and the probability is normalized by a constant $C$ such that:

$$
\int_{0}^{\frac{10}{\lambda_{t}}} C \Sigma_{t} e^{-\Sigma_{\ell} \ell} d \ell=C\left(1-e^{-10}\right)=1
$$

For real geometries, the integral at the interface of the considered case is limited either by defining a vacuum region around it (the neutron leaks out and is lost) or by defining a boundary condition (symmetry, specular reflection, albedo, etc.). A random number $x_{1}$ is sampled from $[0,1]$ to obtain the first path $\ell_{1}$ :

$$
\int_{0}^{\ell_{1}} C \Sigma_{t} e^{-\Sigma_{t} \ell} d \ell=x_{1}
$$

It must be noted that $\ell_{1}$ is a distance travelled in $3 D$ and the projected distance is obtained as $\widetilde{\ell}_{1}=\ell_{1} \sqrt{\cos ^{2} \theta+\sin ^{2} \theta \cos ^{2} \varphi}$. It is now important to determine with which isotope the neutron interacts. The probability of collision with a nuclide $i$ is proportional to its macroscopic contribution to the total cross section $\Sigma_{t}^{i} \equiv N_{i} \sigma_{t}^{i}$. It should be noted that the target isotope must not be chosen only by its mass or isotopic concentration in a medium. The chosen isotope $j \leq p$ is sampled by drawing a random number $x_{\text {target }}$ from [0, 1] such that:

$$
\frac{\sum_{i=1}^{j-1} N_{i} \sigma_{t}^{i}}{\Sigma_{t}}<x_{\text {target }} \leq \frac{\sum_{i=1}^{j} N_{i} \sigma_{t}^{i}}{\Sigma_{t}}
$$

The new question is how to determine the reaction which occurs. Since the total cross section is the sum of the scattering and absorption cross section, a random variable is sampled from $[0,1]$ to decide the interaction type after normalizing it to the total cross section. Using the same logic, the total cross section can be decomposed into a finite number of different interactions (Fig. 9.22).

If the sampled reaction is absorption, the neutron path stops and a new particle is sampled from the source.

The next question consists in knowing the energy to which the neutron is slowed down after its collision during scattering, and in which direction, it is re-emitted. From the slowing-down theory, the slowing-down probability from energy $E$ to energy $E_{k}$ by a target with one atom is given by the flat distribution between $E_{k}$ and the minimum energy that can be reached $\alpha_{i} E_{k}$ :

$$
P(E) d E=\frac{d E}{E_{k}\left(1-\alpha_{i}\right)} \quad \text { with } \quad \alpha_{i}=\left(\frac{A_{i}-1}{A_{i}+1}\right)^{2}
$$

Fig. 9.22 Random sampling of the interaction type


Then, the random variable $x_{k+1}$ can be sampled from $[0,1]$ to calculate $E_{k+1}$ after the collision such that:

$$
x_{k+1}=\int_{E_{k+1}}^{E_{k}} P(E) d E=\frac{E_{k}-E_{k+1}}{E_{k}\left(1-\alpha_{i}\right)}
$$

During the thermalization phase, the calculation is more complex and is beyond the scope of this work. It requires knowing the differential scattering cross sections and can be computed for simple cases (free gas model), becoming very complex if chemical bonds between are accounted for. ${ }^{65}$ The previous process is repeated for the next path until the neutron is absorbed.

As for the emission direction of the neutron, it can be supposed that if scattering is isotropic in the laboratory reference frame (which is acceptable for elastic scattering at low energy), the angles $\varphi$ and $\theta$ must be sampled in $3 D$ from $[0,2 \pi]$ and $[0, \pi]$ respectively. For more generality, scattering can be assumed to be isotropic in the center of mass reference frame and the cosine of the scattering

[^228]
angle $\mu_{k}$ is sampled randomly in that frame. If $\Psi$ is the latter angle, in the range $[0, \pi]$, the scattering probability for that angle which is equiprobable with the other angle by rotation about the incident $\vec{\Omega}$ axis, is written as:
$$
P(\Psi) d \Psi=\frac{d \Omega}{4 \pi}=\frac{2 \pi r^{2} \sin \Psi d \Psi}{4 \pi r^{2}}=\frac{\sin \Psi}{2} d \Psi
$$

Due to the possible variations of angle $\Psi$, this probability is positive and its integral over $[0, \pi]$ is equal to 1 . Therefore, a random variable $x_{\Psi}$ is sampled in $[0,+1]$ and such that:

$$
x_{\Psi}=\int_{-1}^{\mu_{k}} \frac{\sin \Psi}{2} d \Psi=\frac{1+\mu_{k}}{2}
$$

This approach is equivalent to randomly choosing $\mu_{k}=\cos \Psi_{k}$ in $[-1,+1]$. Then, from $\mu_{k}=\cos \Psi_{k}$, the angle $\theta_{k}$ can be deduced in the laboratory frame using the formula for the composition of velocities as discussed in the chapter on slowingdown. The neutron energy after slowing-down is given by the following formula:

$$
E_{k+1}=E_{k}\left(\frac{\left(1+\alpha_{i}\right)+\left(1-\alpha_{i}\right) \mu_{k}}{2}\right)
$$

If scattering is not isotropic in the center of mass frame itself, the scattering probability (i.e. the differential scattering cross section) is expanded on Legendre polynomials $P_{l}(\mu)$ :

$$
p(E, \mu)=\sum_{l=1}^{n} \frac{2 l+1}{2} p_{l}(E) P_{l}(\mu)
$$

$\mu_{k}$ is evaluated as:

$$
\int_{-1}^{\mu_{k}} p(E, \mu) d \mu=x_{\Psi}
$$

It should be noted that scattering does not occur in the plane itself, hence explaining why two angles are chosen: the azimuthal angle $\varphi$ assumed to be uniformly distributed in $[0,2 \pi]$, and the other angle known by other velocity triangle (from the composition of velocity vectors) and depending only on $\mu_{k}$. Finally, the projection of the leakage direction in the plane is calculated just as for the incident angle. In the case of a heterogeneous medium in $2 D$, space in our

Fig. 9.23 Paving plane space into homogeneous zones

illustration as being regular along $x$ and $y$ (Fig. 9.23) for didactic simplicity, ${ }^{66}$ is paved into zones. Each zone is assumed to be homogeneous.

In the case of a uniformly-distributed source in the homogeneous medium, the starting-point of neutrons is obtained by drawing two random variables: $x_{0}$ in $[x(1)$, $x(m)]$ and $y_{0}$ in $[y(1), y(n)]$. Given that the compositions $j$ can be different (each zone has a unique composition $(m, n)$ ), the slowing-down density of neutrons below energy $E_{k}$ due to the material constitution of $j$ is given by:

$$
q_{j}=\sum_{i \in j} N_{j}^{i} \xi_{i} \sigma_{s}^{i}
$$

The contribution of the composition of $j w r t$ the other compositions is obtained by integrating the density over the surface of the composition $j$, i.e. $q_{j} A_{j}$ where $A_{j}$ is the area of the zones with composition $j$ :

$$
A_{j}=\sum_{(m, n)=j}\left(x_{m+1}-x_{m}\right)\left(y_{n+1}-y_{n}\right)
$$

Using the normalized densities defined as:

$$
Q_{j}=\frac{q_{j} A_{j}}{\sum_{k} q_{k} A_{k}}
$$

[^229]The initial composition is obtained by seeking the composition $k$ such that, from the random variable $x_{\text {compo }}$ sampled from [0,1]:

$$
\sum_{j=1}^{k} Q_{j}<x_{\text {compo }} \leq \sum_{j=1}^{k+1} Q_{j}
$$

The initial region $\left(m_{k}, n_{k}\right)$ is then reached by normalizing the contribution of each region with composition $k$ to the slowing-down density, i.e. by drawing a random variable $x_{m, n}$ in the $[0,1]$ interval:

$$
\left\{\begin{array}{l}
Q_{m, n}^{k}=\frac{A_{m, n}^{k} q_{k}}{\sum_{(m, n)=k} A_{m, n}^{k} q_{k}} \\
\sum_{m=1}^{m_{k}-1} \sum_{n=1}^{n_{k}-1} Q_{m, n}^{k}<x_{m, n} \leq \sum_{m=1}^{m_{k}} \sum_{n=1}^{n_{k}} Q_{m, n}^{k}
\end{array}\right.
$$

The point-source will be precisely determined by drawing a random variable $x_{S}$ from the $\left[x\left(m_{k}\right), x\left(m_{k+1}\right)\right]$ interval and $y_{S}$ from the $\left[y\left(n_{k}\right), y\left(n_{k+1}\right)\right]$ interval. The calculations would be simplified if the composition were assumed different in each zone. It should be noted that the positions of the sources are determined with much difficulty in Monte Carlo for complex geometries. For instance, it can be noted that positioning points homogeneously in a sphere requires the generation of random points in a surrounding cube and then determining if the points (generated by three random variables along the three Cartesian axes) are encompassed in the sphere or not. In fact, the use of the spherical reference frame for that geometry, associated to the random variables with the radius and two angles in the frame, leads to a non-homogeneous distribution.

The interface problem can be solved by an efficient ray-tracing method. In 3D, the calculation of form factors of a volume wrt a point can be simplified significantly by inscribing that volume in a simpler volume for which the solid angle can be evaluated analytically. The analytical work of S. Cramer ${ }^{67}$ provides the analytical solid angles for an impressive amount of particular geometries. They are very useful for determining if a direction may intercept any volume. They can be used in a rejection criterion method to ignore unnecessary paths. When the scattering direction is determined, at least one surface or boundary surface may be intercepted. In the case of an internal interface of the geometry, the variation of the total cross section in the optical path must be accounted to evaluate the next collision point. It must be noted that it is more efficient to sample randomly a path with the same incident direction in the neighboring cell over again rather than

[^230]Fig. 9.24 Boundary conditions of the domain

summing the optical path. If a boundary surface is reached, void boundary conditions would lead to the loss of the neutron. Translation conditions will cause the neutron to appear with the same incident direction on the opposite face of the geometry, while specular reflection repositions the neutron according to the Descartes law of reflection (Fig. 9.24).

### 9.19.3 Statistical Error

The error on the mean values of interest (flux, reaction rate, etc.) can be estimated by fractioning the large number $N$ into $L$ batches of size $N / L$ neutrons rather than studying a large number of trajectories. The values of physical quantities are averaged for each batch and a global mean is computed over all the batches. The empirical variance is thus obtained as an estimation of the calculation precision.

$$
V=\frac{1}{L-1} \sum_{l=1}^{L}\left(X_{l}-\bar{X}\right)^{2} \quad \text { with: } \quad X_{l}=\frac{L}{N} \sum_{n=1}^{N / L} X_{n} \text { and } \bar{X}=\frac{1}{L} \sum_{l=1}^{L} X_{l}
$$

### 9.19.4 Calculation of Physical Quantities

Usually, the flux or the reaction rate in a given region is sought. A weight is defined such that it represents the contribution of the particle wrt all the particles sampled. The initial weight $\omega_{0}$ is 1 and varies for each event undergone by the particle. If the same recurrence is applied to the weights as those on the collision rate, i.e. (Métivier 2006, p. 319):

Table 9.1 Expression of the main estimators for physical quantities of interest

| Estimator | Flux | Reaction rate | Current |
| :--- | :--- | :--- | :--- |
| Chord per volume | $\omega \ell$ | $\omega \ell \Sigma_{i}$ |  |
| Collision per volume | $\omega / \Sigma_{t}$ | $\omega \Sigma_{i} / \Sigma_{t}$ |  |
| Surface quantity | $\omega /(\vec{\Omega} \cdot \vec{n})$ |  | $\omega$ |

$$
\omega_{1}=\omega_{0} \int_{D} S\left(P_{1}\right) d P_{1}
$$

following the process that consists in positioning a neutron at a point-source $P_{1}$ of the phase space $D$ according to the function $S\left(P_{1}\right)$ (in practice, the position, energy, and direction of the source-neutron are sampled). The collision rate at the initial energy is equal to the source. Then, the weights are propagated using the Peierls collision operator:

$$
\omega_{n}=\omega_{n-1} \int_{D} K\left(P_{n-1} \rightarrow P_{n}\right) d P_{n-1}
$$

after each collision. The random variable $\omega_{n}$ is thus an estimator of the collision rate and $E\left(\omega_{n}\right)=\Sigma_{t} \Phi_{n}$. If the values of the estimator $\omega_{n}$ in a given volume are scored, the rate of the nth collision in that volume is obtained. For $N$ particles sampled (Table 9.1):

$$
\Sigma_{t} \Phi_{n} \approx \frac{1}{N} \sum_{i=1}^{N} \omega_{n}^{i} \quad \text { and } \quad \Sigma_{t} \Phi \approx \sum_{n=1}^{\infty} \Sigma_{t} \Phi_{n}
$$

### 9.19.5 Generalization, Biasing

For the general case of fission sources, the flux is required to obtain the source positions so an initial guess is required. In practical situations, the localization of sources is deemed known initially and a number of neutrons are sampled to calculate the real sources, thence ignoring these cycles in the statistics according to the problem being solved and the geometrical coupling among sources. The biasing method is employed in non-analogue simulations for cases where the true physical law of probability distribution are not used, e.g. by choosing a preferential emission direction. ${ }^{68}$ A weight $w$ is given to the neutron, which implies that it is no longer a single neutron but rather a beam of neutrons of which the weight represents

[^231]the intensity. Hence, the initial weight is 1 and at each collision, it is considered that a fraction of the beam is absorbed by multiplying the weight by $1-\Sigma_{a} / \Sigma_{t}$, meaning that the weight decreases in an absorbing medium. Unlike analogue simulation where the neutron is ignored after its absorption, the simulation continues as if the neutron survived the collision and its statistical weight is diminished. A threshold $s$ is predefined and is used conditionally to ignore any neutron with a contribution that is too low, and for which continuing the path would be useless. If $w<s$, the final weight is multiplied by $1 / s$ and the neutron with a probability $s$ is left out, which is physically equivalent to grouping low-intensity beams by conserving their total contribution at the expense of computational time. Similarly, the ratio $\nu \Sigma_{f} / \Sigma_{t}$ gives a fission reaction. During collisions, a fission neutron is selected for the next step with probability of $w \nu \Sigma_{f} / \Sigma_{t}$ (Criticality control of fissile materials 1968, p. 137). The multiplication coefficient, for criticality applications, is obtained by summing over all the collisions for all the simulated neutrons, i.e. the various values of $w \nu \Sigma_{f} / \Sigma_{t}$. Another concrete example can be illustrated with the fluence of the reactor vessel which determines the damage of the steel of the reactor vessel by fast neutrons (Interaction radiation solids 1964). Physically, only fast neutrons leaking from the core have a probability of reaching and thereby, damaging the vessel which is protected by water and steel. The fission neutrons with energy lower than 1 MeV have almost no chance of reaching it. Thus, it seems wise in that example not to simulate neutrons in the complete energy spectrum but only those with energy values above 1 MeV . The calculation is thus biased. Another approach called the Russian roulette method (Spanier and Gelbard 1969, p. 124), consists in ignoring neutrons that are in an uninteresting part of the phase space ("wrong" directions, too low energy, etc.) for the required score by modifying the weight of surviving particles such that the expectation of the weight remains unchanged. Hence, a probability $p$ is given to the weights of neutrons for which the simulation continues, and $1-p$ for those which are ignored. With the same logic, a particle in an interesting part of the phase space can be split (Clark and Hansen 1964, p. 272), (Spanier and Gelbard 1969, p. 125). For fluence problems, the flux level is only of $710^{10} \mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}$, and it is complicated to transport neutrons that far from the core, thereby explaining why $45 \%$ of the neutrons reaching the reactor vessel originate from assemblies that are at the end of the assembly line that is closer to the vessel, and that assemblies that are further way do not contribute to fluence. Furthermore, as the neutron draws closer to the vessel, it is also interesting to assume that a fictitious neutron has followed strictly the same direction as the reference neutron and allowing both neutrons to live on randomly. Indeed, the weights are modified so as to conserve the initial weight. This logic has a limit for precision given that it is not sensible to split a neutron indefinitely as it closes on its target just to avoid sampling neutrons from the core, given that all the neutrons created (with a correspondingly low weight) have exactly the same history, and may cause problems of statistical independence. This process would be somehow equivalent to calculating the flux on the reactor vessel using only one fission neutron! Similarly, to calculate the flux on a precisely-known target (a detector), it is wise to bias the simulation by using the adjoint flux due to that detector if it can be easily calculated
(e.g. via a deterministic calculation that could provide that quantity ${ }^{69}$ ). The following paragraphs illustrate techniques for improving counting for a detector.

### 9.19.6 Resonance Escape Probability Factor Calculation

The first use of the Monte Carlo method in neutron physics in France is attributed to Régis Eyraud ${ }^{70}$ whose doctoral work in 1967 was based on the calculation of the resonance escape probability factor and epithermal resonant absorption for slab reactors such as those used for naval propulsion (submarines). The fuel is a lattice of boxes containing slab fuel, and the absorbing materials have cross shapes with hafnium. The geometry is too complex for the analytical codes of the time (ZUT, GAROL) and required approximations on the lattice properties. Besides, the equivalent US code RECAP conceived by Westinghouse at the Bettis Laboratory was not available in France.

In these pioneering calculations, a neutron is generated by assuming that the flux was flat spatially, with a $1 / E$ spectrum, and the neutron history is generated by random sampling according to the strategy that has been discussed earlier. If $n$ is the

[^232]
total number of neutrons that are simulated, $a$, the number of absorbed neutrons during slowing down, the resonance escape probability factor is given by:
$$
p=1-\frac{a}{n}
$$

If the neutron is absorbed, the count is 0 , otherwise if it survives resonant captures, 1 . Therefore, the variance is calculated as:

$$
\sigma_{n}=\frac{a(1-a)}{\sqrt{n}}
$$

It can be noted that $p$ can be obtained as a function of energy via an adequate storing of capture data during slowing-down. Similarly, the spatial distribution of absorption can also be computed, as well as the isotopic distribution. These results are statistically more uncertain since the number of events in one zone is considerably smaller than the calculation of the resonance escape probability factor for the whole geometry.

In such calculations, the calculation of the resonance escape factor for neutrons reaching a very low energy can be carried out by improving the computational "efficiency" through biasing. The latter consists in never ignoring an absorbed neutron so as not to lose the history already calculated. If random sampling leads to the absorption of a neutron, its weight is reduced by a factor of $\Sigma_{a} / \Sigma_{t}$, and the simulation goes on. If the neutron weight is $w$ before the absorbing collision, it changes to $w \Sigma_{a} / \Sigma_{t}$ after the pseudo-absorption, while remaining unchanged if the sampled reaction is scattering. Since the isotope by which the neutron is absorbed is not known, this absorption is proportionally distributed according to the contribution of each isotope to the absorption rate. This biasing technique reduces the variance of the resonance escape factor by 2 at the expense of the increase in the processing of neutron simulations since each history lasts globally longer. This is why neutrons with low weights are ignored since they do not significantly contribute to the required response. The weight of an ignored neutron is added to the weight of the next emitted neutron in the same energy range (thereby conserving the total weight of emitted neutrons in an energy group). Finally, the absorption rate in group $g$ is given by:

$$
R_{a, g} \equiv \int_{E_{g+1}}^{E_{g}} \Sigma_{a}(E) \Phi(E) d E \approx \xi_{c}=\sum_{i=0}^{c}\left(\frac{\Sigma_{a}}{\Sigma_{t}}\right)_{x_{i}} w_{i}
$$

where $x_{i} \equiv\left(\vec{r}_{i}, \overrightarrow{\Omega_{i}}, E_{i}\right)$ represents the neutron position in the phase space, $w_{i}$ is the neutron weight after $i$ collisions and $c$ the number of collisions in group $\left[E_{g+1}, E_{g}\right.$ ] (the energy groups are indexed in decreasing order as usual). If $n$ is the total number of simulated neutron histories:

$$
a=E(\xi)=\sum_{k=1}^{n} \frac{\xi_{k}}{n} \quad \text { and } \quad p=1-a
$$

Hence, we obtain the calculation of the estimated value $E(\xi)$ of the absorption probability. The question of the confidence of that result remains. A simple strategy which does not require any additional history simulation consists in artificially dividing the total history number $n$ into $p$ packets of $m$ histories, i.e.:

$$
n=m q
$$

$p$ new quantities are defined as

$$
\xi^{i}=\frac{1}{m} \sum_{k=1}^{m} \xi_{k}^{i} \quad i=1, \ldots, p
$$

The $\xi^{i}$ are simply attempts at evaluating $\xi$ for a reduced number of histories. If $m$ is large enough, the $\xi^{i}$ have a normal distribution according to the central limit theorem, the distribution being more regular as the number of packets $p$ gets larger. The expectation of each $\xi^{i}$ is still $E(\xi)$. Let us define:

$$
\overline{\xi^{p}} \equiv \frac{1}{p} \sum_{k=1}^{p} \xi^{k} \quad \text { and } \quad s_{\xi}^{2} \equiv \frac{1}{p} \sum_{k=1}^{p}\left(\xi^{k}\right)^{2}-\left(\frac{1}{p} \sum_{k=1}^{p}\left(\xi^{k}\right)\right)^{2}
$$

then, the probability theory indicates that the random variable:

$$
t=(p-1)\left(\frac{\overline{\xi^{p}}-E(\xi)}{S_{\xi}}\right)
$$

is given by a Student distribution with $p-1$ degrees of freedom for the random variable $t$ if the packet number $p$ is large enough. This concept of subdividing the total number of histories into packets of the same size gives a range for the mathematical expectation being solved for. Therefore, the probability that the estimated value be in a determined interval is approximated by the Student integral:

$$
P\left(\overline{\xi^{p}}-\frac{b s_{\xi}}{p-1} \leq E(\xi) \leq \overline{\xi^{p}}-\frac{a s_{\xi}}{p-1}\right) \approx \int_{t=a}^{t=b} s_{p-1}(t) d t
$$

It is thus a simple means of evaluating the precision of the estimated value using the individual packet data.

Fig. 9.25 Direct Monte
Carlo simulation


Fig. 9.26 Reverse Monte Carlo simulation


### 9.19.7 Midway Monte Carlo

The difficulty of transporting neutrons in a required region by direct simulation decreases the quality of the statistics for a detector response (Fig. 9.25). I.V. Serov proposed ${ }^{71,72}$ an approach called the midway Monte Carlo which uses an interesting domain decomposition property of the Boltzmann equation. A direct simulation consists in sampling neutrons directly from the source and tallying those that reach the detector (Fig. 9.26). Hence the direct flux is calculated as well as its associated detector response (usually the absorption rate).

The adjoint simulation consists in simulating the neutron trajectories starting from the detector with an associated adjoint source corresponding to the desired response function and the neutron history is tracked backwards up to the true source (Fig. 9.26). The equations satisfied by the flux and the adjoint flux are as follows (Spanier and Gelbard 1969, p. 169):

[^233]$\left\{\begin{array}{c}\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega}, E)+\Sigma_{t}(\vec{r}, \vec{\Omega}, E) \Phi(\vec{r}, \vec{\Omega}, E)-\int_{\vec{\Omega}} d \vec{\Omega} \prime \int_{E^{\prime}} d E^{\prime} \Sigma_{s}\left(\vec{r}, \vec{\Omega} \prime \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, \vec{\Omega} \prime, E^{\prime}\right)=S(\vec{r}, \vec{\Omega}, E) \\ -\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}(\vec{r}, \vec{\Omega}, E)+\Phi^{*}(\vec{r}, \vec{\Omega}, E) \Sigma_{t}(\vec{r}, \vec{\Omega}, E)-\int_{\vec{\Omega}} d \overrightarrow{\Omega^{\prime}} \int_{E^{\prime}} d E^{\prime} \Phi^{*}(\vec{r}, \vec{\Omega}, E) \Sigma_{s}\left(\vec{r}, \vec{\Omega} \rightarrow \vec{\Omega}, E \rightarrow E^{\prime}\right)=S^{*}(\vec{r}, \vec{\Omega}, E)\end{array}\right.$
which are expressed more concisely with the absorption operator without the gradient term:

$$
\begin{gathered}
\left\{\begin{array}{l}
A_{\vec{\Omega}, E}[] \equiv\left(\Sigma_{t}-\int_{\vec{\Omega}} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} \Sigma_{s}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right)\right)[] \\
A_{\vec{\Omega}, E}^{*}[] \equiv\left(\Sigma_{t}-\int_{\vec{\Omega}} d \vec{\Omega} \int_{E^{\prime}} d E^{\prime} \Sigma_{s}\left(\vec{r}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}, E \rightarrow E^{\prime}\right)\right)[]
\end{array}\right. \\
\left\{\begin{array}{l}
\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega}, E)+A_{\vec{\Omega}, E}[\Phi(\vec{r}, \vec{\Omega}, E)]=S(\vec{r}, \vec{\Omega}, E) \\
-\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi^{*}(\vec{r}, \vec{\Omega}, E)+A_{\vec{\Omega}, E}^{*}\left[\Phi^{*}(\vec{r}, \vec{\Omega}, E)\right]=S^{*}(\vec{r}, \vec{\Omega}, E)
\end{array}\right.
\end{gathered}
$$

The adjoint equation is different from the direct equation with the presence of the "-" sign in front of the streaming term and the transposition of the scattering term. The operator $A_{\Omega_{, E}}[]$ is not self-adjoint since $A_{\Omega_{, E}}[] \neq A_{\Omega_{, E}}^{*}$ []. However, their double integration over energy and angle are equal:

$$
\int_{\vec{\Omega}} d \vec{\Omega} \int_{E} d E \Phi^{*} A_{\vec{\Omega}, E}[\Phi]=\int_{\vec{\Omega}} d \vec{\Omega} \int_{E} d E \Phi A_{\vec{\Omega}, E}^{*}\left[\Phi^{*}\right]
$$

The total detector response is given by both formulations:

$$
\left\{\begin{array}{l}
R=\iint_{E} \int_{\vec{\Omega} V} S^{*}(\vec{r}, \vec{\Omega}, E) \Phi(\vec{r}, \vec{\Omega}, E) d \vec{r} d \vec{\Omega} d E \\
R=\int_{E} \int_{\vec{\Omega}} \int_{V} \Phi^{*}(\vec{r}, \vec{\Omega}, E) S(\vec{r}, \vec{\Omega}, E) d \vec{r} d \vec{\Omega} d E
\end{array}\right.
$$

Let us consider an arbitrary domain $V_{\text {mid }}$, of surface $\partial V_{\text {mid }}$, which contains the detector but not the source. It is called the midway volume even if the surface of that volume is not strictly halfway from the source (Fig. 9.27). Two simulations are considered: the first one is direct and stops at the boundary surface $\partial V_{\text {mid }}$, thereby tallying the incoming flux at that surface. The second one is adjoint, carried out as the previous one but from the inside to calculate the adjoint flux on that surface.

The direct equation is multiplied by $\Phi^{*}(\vec{r}, \vec{\Omega}, E)$, and the adjoint equation by $\Phi(\vec{r}, \vec{\Omega}, E)$, then both equations are integrated term-wise over the space

Fig. 9.27 Monte-Carlo at midway

represented by the volume $V_{\text {mid }}$, over energy and angle. The resulting equations are subtracted term-wise:

$$
\left\{\begin{array}{r}
\iint_{E} \int_{\vec{\Omega} V_{\text {mid }}}\left(\Phi^{*}(\vec{r}, \vec{\Omega}, E) \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega}, E)+\Phi^{*}(\vec{r}, \vec{\Omega}, E) A_{\vec{\Omega}, E}[\Phi(\vec{r}, \vec{\Omega}, E)]\right) d \vec{r} d \vec{\Omega} d E \\
=\iint_{E} \int_{\vec{\Omega} V_{\text {mid }}} S(\vec{r}, \vec{\Omega}, E) \Phi^{*}(\vec{r}, \vec{\Omega}, E) d \vec{r} d \vec{\Omega} d E \\
\iint_{E} \int_{\vec{\Omega} V_{\text {mid }}}\left(-\Phi(\vec{r}, \vec{\Omega}, E) \vec{\Omega} \cdot g r a d \Phi^{*}(\vec{r}, \vec{\Omega}, E)+\Phi(\vec{r}, \vec{\Omega}, E) A_{\vec{\Omega}, E}^{*}\left[\Phi^{*}(\vec{r}, \vec{\Omega}, E)\right]\right) d \vec{r} d \vec{\Omega} d E \\
=\iint_{E} \int_{\vec{\Omega}} S_{\text {Vid }} S^{*}(\vec{r}, \vec{\Omega}, E) \Phi(\vec{r}, \vec{\Omega}, E) d \vec{r} d \vec{\Omega} d E
\end{array}\right.
$$

For concision, the scalar product is denoted as:

$$
\langle f, g\rangle_{V} \equiv \int_{E} \int_{\vec{\Omega}} \int_{V} f(\vec{r}, \vec{\Omega}, E) g(\vec{r}, \vec{\Omega}, E) d \vec{r} d \vec{\Omega} d E
$$

The term-wise subtraction leads to:

$$
\left\langle\Phi^{*} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi+\Phi \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}\right\rangle_{V_{\text {mid }}}=\left\langle S \Phi^{*}\right\rangle_{V_{\text {mid }}}-\left\langle S^{*} \Phi\right\rangle_{V_{\text {mid }}}
$$

Since the direct source is outside $V_{\text {mid }},\left\langle S \Phi^{*}\right\rangle_{V_{\text {mid }}}=0$. Furthermore, the Ostrogradski theorem transforms the volume integral as a surface integral:

$$
\begin{aligned}
\left\langle\Phi^{*} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi+\Phi \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi^{*}\right\rangle_{V_{\text {mid }}} & =\left\langle\vec{\Omega} \cdot \overrightarrow{g r a d}\left(\Phi \Phi^{*}\right)\right\rangle_{V_{\text {mid }}} \\
& =\int_{\partial V_{\text {mid }}} \vec{n} \cdot \vec{\Omega} \Phi \Phi^{*} d^{2} r
\end{aligned}
$$

Therefore, the detector response is expressed as follows, while noting that the adjoint source is zero outside $V_{\text {mid }}$ :

$$
R=\left\langle S^{*} \Phi\right\rangle_{V_{\text {mid }}}=-\int_{\partial V_{\text {mid }}} \vec{n} \cdot \vec{\Omega} \Phi \Phi^{*} d^{2} r
$$

The surface integral on the right contains the term of incoming neutron current: $J=-\vec{n} . \vec{\Omega} \Phi$ which is stored in the direct simulation and multiplied by the adjoint flux computed on the surface by the adjoint simulation. This method leads to the decoupling of the problem through the calculation of the direct and adjoint problems with satisfactory statistics without requiring neutron transport to the source or the detector, assuming that the surface is wisely chosen. The method can be extended to coupled neutron-photon transport to obtain the photon response of the detector. In this case, by indexing the neutron equations by $n$ and the photon ones by $p$, and by denoting the photon productions by neutrons as $P$, the following equations are reached:

$$
\left\{\begin{array}{c}
\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{n}+A_{n}\left[\Phi_{n}\right]=S \\
-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{n}^{*}+A_{n}^{*}\left[\Phi_{n}^{*}\right]=P^{*} \\
\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{p}+A_{p}\left[\Phi_{p}\right]=P \\
-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi_{p}^{*}+A_{p}^{*}\left[\Phi_{p}^{*}\right]=S^{*}
\end{array}\right.
$$

In these expressions, $S^{*}$ is the photon response function of the detector and $R=\left\langle S^{*} \Phi\right\rangle_{V}$ is the integrated response. $A_{n}[] \equiv\left(\Sigma_{t}-\int \Sigma_{s} d E\right)$ [ ] is the direct absorption operator and the other $A\left[\right.$ ] operators are deduced from that definition, $P^{*}$ is the adjoint source function of neutrons produced by adjoint photons:

$$
\left\{\begin{array}{l}
P=\int_{\vec{\Omega}^{\prime}} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} \Sigma_{\text {produc }}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, E^{\prime} \rightarrow E\right) \Phi_{n}\left(\vec{r}, \vec{\Omega}^{\prime}, E^{\prime}\right) \\
P^{*}=\int_{\vec{\Omega}} d \vec{\Omega}^{\prime} \int_{E^{\prime}} d E^{\prime} \Phi_{p}^{*}\left(\vec{r}, \vec{\Omega}^{\prime}, E^{\prime}\right) \Sigma_{\text {produc }}\left(\vec{r}, \vec{\Omega} \rightarrow \vec{\Omega}^{\prime}, E \rightarrow E^{\prime}\right)
\end{array}\right.
$$

Applying the same integration-subtraction procedure as described earlier, the following equations are finally written:

$$
\left\{\begin{array}{c}
\int_{\partial V_{\text {mid }}} \vec{n} \cdot \vec{\Omega} \Phi_{n} \Phi_{n}^{*} d^{2} r=\left\langle S \Phi_{n}^{*}\right\rangle_{V_{\text {mid }}}-\left\langle P^{*} \Phi_{n}\right\rangle_{V_{\text {mid }}} \\
\int_{\partial V_{\text {mid }}} \vec{n} \cdot \vec{\Omega} \Phi_{p} \Phi_{p}^{*} d^{2} r=\left\langle P \Phi_{p}^{*}\right\rangle_{V_{\text {mid }}}-\left\langle S^{*} \Phi_{p}\right\rangle_{V_{\text {mid }}}
\end{array}\right.
$$

From the definition of $P$ and $P^{*}$, and for any volume, $\left\langle P^{*} \Phi_{n}\right\rangle_{V}=\left\langle P \Phi_{p}^{*}\right\rangle_{V}$, thereby leading to the following equation by adding the equations term-wise, and since $\left\langle S \Phi_{n}^{*}\right\rangle_{V_{\text {mid }}}=0$ :

$$
R=\left\langle S^{*} \Phi_{p}\right\rangle_{V_{\text {mid }}}=-\left(\int_{\partial V_{\text {mid }}} \vec{n} \cdot \vec{\Omega} \Phi_{n} \Phi_{n}^{*} d^{2} r+\int_{\partial V_{\text {mid }}} \vec{n} \cdot \vec{\Omega} \Phi_{p} \Phi_{p}^{*} d^{2} r\right)
$$

The result is very similar to the neutron transport problem.

### 9.19.8 Quasi-Deterministic Approximation of the Importance Function

An efficient means of biasing Monte Carlo calculations is the use of the adjoint flux or the importance which is calculated through reverse simulations. Nevertheless, the problem of the statistical precision of the importance function remains when few particles are scored in a given volume. One way of solving that problem is by the calculation of the importance function by a deterministic code. The main drawback is that the major advantage of the Monte Carlo method to deal with complex geometries is no longer available. A very elegant method ${ }^{73}$ to calculate the importance function with better precision while retaining the advantages of the Monte Carlo method is the quasi-deterministic approximation. The geometry is paved with $n$ media of interest, which are indexed with Roman numerals to avoid any confusion. A discrete transport state corresponds to one of these media to which an energy range in a multi-group approach is associated, along with a path direction. To simplify the illustration, we will consider only one energy group, meaning that a medium has two states: the neutron is travelling either towards the top or the bottom wrt the geometrical orientation. However, it should be noted that the extension to multi-group is possible. In Fig. 9.28, the states 1 to 5 correspond to their respective medium along with the state of a neutron moving "upwards" (symbol $\Uparrow$ ) while the states -1 to -5 correspond to the same medium for neutron with a direction state to the bottom (symbol $\Downarrow$ ).

Let us suppose that ten neutrons are sampled randomly in medium IV with an upgoing path (state $4 \Uparrow$ ) by positioning sources randomly in that medium. The Monte Carlo simulation is then executed for one step in transport, i.e. these neutrons are tracked until their next collision and are ignored afterwards. It can be noted that three processes are possible:

[^234]

Fig. 9.28 Geometry for a quasi-deterministic example

- either there is a scattering which is the most probable physical case (in medium IV or any other),
- or there is an absorption (as in Fig. 9.28 as shown by a dot at the end of the upgoing path)
- or the neutron may stream out from the geometry through the tallying surface located at the top of the figure in the illustrated example where the neutron is given a tally of 1 , or by another surface where the tally is worth 0 .

Consider the path $c$ : the neutron leaves the state $4 \Uparrow$ to enter the medium II where it takes the state $2 \Uparrow$ and is scattered to state $-2 \Downarrow$. Here, the term "leaves" does not characterize the fact of leaving the geometry but undergoing a change of state. Therefore, the table of states of the simulated neutrons with initial state $4 \Uparrow$ can be completed (Table 9.2). From all the simulated neutrons, only the neutron $h$ obtains a

Table 9.2 State table for a one step of quasi-deterministic transport for medium IV

| Source <br> state | Outgoing <br> state | Considered <br> trajectories | Mean weight of the outgoing <br> state per unit source | Tally of <br> the path | Mean <br> score |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $4 \Uparrow$ | $0 \Rightarrow$ | $a, f, h, j$ | $p_{4,0}=\frac{4}{10}$ | $0,0,1,0$ | $s_{4,0}=\frac{1}{4}$ |
| $4 \Uparrow$ | $-4 \Downarrow$ | $g$ | $p_{4,4}=\frac{1}{10}$ | 0 | $s_{4,-4}=\frac{0}{1}$ |
| $4 \Uparrow$ | $-2 \Downarrow$ | $c$ | $p_{4,-2}=\frac{1}{10}$ | 0 | $s_{4,-2}=\frac{0}{1}$ |
| $4 \Uparrow$ | $-1 \Downarrow$ | $d, i$ | $p_{4,-1}=\frac{2}{10}$ | 0,0 | $s_{4,-1}=\frac{0}{2}$ |
| $4 \Uparrow$ | $1 \Uparrow$ | $e$ | $p_{4,1}=\frac{1}{10}$ | 0 | $s_{4,1}=\frac{0}{1}$ |
| $4 \Uparrow$ | $-5 \Downarrow$ | $b$ | $p_{4,-5}=\frac{1}{10}$ | 0 | $s_{4,-5}=\frac{0}{1}$ |

tally of 1 since it crosses the tallying surface. The "sterile" probability of the state transfer $p_{i, j}$ normalized to the source can thus be calculated. It is equivalent to the number of neutrons reaching a state $j$ divided by the total number of simulated neutrons. In a non-multiplying medium, it is the probability to pass from state $i$ to state $j$. On the other hand, for a multiplying medium, the exact probability to pass from state $i$ to state $j$ must allow for the new fission neutrons (a priori, if fission is isotropic, $\nu / 2$ travel upwards and the same amount to the bottom, $\nu$ being an integer value sampled randomly in the probability distribution for the production of fission neutrons). It is thus different from the definition of $p_{i, j}$ that is employed. Similarly, the mean score $s_{i, j}$ is computed by tallying the scores 1 or 0 according to the fact that the neutron travels through the tallying surface or not. The score averaged over the inverse history (as for the adjoint flux), i.e. the importance $I_{i}$, can be calculated by noting that this score is equal to that of the next events to which the scores of all the subsequent events are added. This recurrence over time is expressed as:

$$
\begin{equation*}
\text { Recurrence equation for the importance function: } \quad I_{i}=\sum_{j} p_{i, j} s_{i, j}+\sum_{j} p_{i, j} I_{j} \tag{9.49}
\end{equation*}
$$

Picture 9.210 cycles


This linear system with $J=2 n+1$ unknowns allows the calculation of the importance function of each medium relative to the tallying surface. Booth points out that the method is independent of the biasing method used for calculating $p_{i, j}$ and $s_{i, j}$, only the numerical values of these quantities vary. Besides, simulations with two steps can be considered, i.e. tracking neutrons for two successive collisions, or even more. Thus, neutrons can be transported towards the tallying surface for convenient considerations without debunking Eq. (9.49) which remains valid for the corresponding numerical values of $p_{i, j}$ and $s_{i, j}$. For multi-group cases, the media are replaced by regions that are composed of one given energy group for a given physical medium. The phase space contains a supplementary dimension but the formalism remains valid.

### 9.19.9 Example of a Monte Carlo Calculation

To illustrate this section, we present a Monte Carlo simulation (with the French TRIPOLI code from $C E A$ ) that depicts the total flux created by a unit source placed

Picture 9.3100 cycles


Picture 9.41000 cycles. Calculations by Sylvain Rollet, EDF (2009)

at the center of the reactor. The calculation is carried out for an $1 / 8$ th of the core thanks to symmetry considerations. Between each photograph, the number of cycles with 10,000 particles is multiplied by 10 (Pictures 9.2, 9.3, and 9.4).

The neutron transport in the multiplying medium can thus be visualized by the increase of the flux in the core. On the last picture, pseudo-square zones that are darker can be observed in the active core. They correspond to fresh (non-depleted) assemblies where the flux is higher (in red). The dark zone at the periphery on the top of the photograph is in fact a zone with low flux (in blue).

## Part II <br> Reactor Physics

# Chapter 10 <br> Diffusion Approximation in Neutron Physics 

### 10.1 Fick's Law

In 1851, Adolph Eugen Fick (1829-1901), a German ophthalmologist (Photo 10.1), postulated intuitively the relationship between a chemical concentration flux and its gradient in a solution by analogy with Fourier's law in heat conduction. It was only 50 years later that Albert Einstein demonstrated the accuracy of Fick's law through his work on Brownian motion. In neutron physics, a neutron scatters through matter with successive collisions that reduce its energy to thermal energy, whence the analogy with collisions of non-interacting molecules in a gas. The free scattering path is the sum of the elementary distances covered by the neutron between each collision (with atoms that constitute matter) from its birth till its loss through absorption (length of the dotted line in Fig. 10.1). The mean free scattering path $\lambda_{s}$ is the mean distance normalized to one collision. It is obtained by dividing the free scattering path by the number of collisions.

### 10.1.1 Evaluation of the Neutron Diffusion Coefficient

(Reuss 2003, p131)
Fick's law linearly relates a physical quantity to its derivative. It formulates the idea that a quantity diffuses in the direction of its gradient in the same way that salt in salted water diffuses from zones of higher concentration to zones of lower concentration or that heat transfers from hotter zones to cooler ones. Applying this relation to neutron physics, the relation between the neutron current and its flux is similar to that which exists in the heat equation between the temperature field and


Fig. 10.1 $3 D$ neutron diffusion and collisions in matter before radiative capture


Photo 10.1 Adolph Fick invented the first contact lenses. His name remains nevertheless associated with the two Fick's laws
the heat flux. The demonstration is based on various physical quantities that must be mentioned:

- We consider an infinite medium that is fairly uniform (the total cross section $\Sigma_{t}$
( $\vec{r}$ ) varies weakly around $\vec{r}$ )
- There is no point neutron source in the medium
- Scattering is isotropic in the laboratory frame, i.e. $\Sigma_{s}\left(\vec{r}, \vec{\Omega}^{\prime} \rightarrow \vec{\Omega}, v, t\right)=$ $\frac{1}{4 \pi} \Sigma_{s}(\vec{r}, v, t)$;
- The flux varies slowly with position $\vec{r}$ (a first-order Taylor expansion can be used around a given point).

Let us consider a given point as the origin of Cartesian coordinates $(x, y, z)$ in which the scalar currents $J_{x}, J_{y}$ and $J_{z}$ are the components of current vector $\vec{J}$. Let us now compute the current $J_{z}$ using the directional contributions $J_{z}^{-}$and $J_{z}^{+}$of the neutron moving from the hemisphere $z>0$ to that in which $z<0$, and conversely. In the absence of sources, any neutron passing by the origin comes from point $\vec{r}$ at which it underwent scattering. The scattering reaction rate at $\vec{r}$ is given by $\Sigma_{s}(\vec{r}, v, t) \Phi(\vec{r}, v, t)$. Since diffusion is assumed to be isotropic, the number of scattered neutrons from point $\vec{r}$ to the surface element $d S_{z}$ (in the $x O y$ plane in Fig. 10.2, close to the origin) is the product of the scattering reaction rate at time $t-r / v$, where $v$ is the speed of the neutron, multiplied by the solid angle of the surface element as seen from the initial point $\vec{r}$ :
$\Sigma_{s}\left(\vec{r}, v, t-\frac{r}{v}\right) \Phi\left(\vec{r}, v, t-\frac{r}{v}\right) \frac{\vec{\Omega} \cdot \overrightarrow{d S_{z}}}{4 \pi r^{2}}=\Sigma_{s}\left(\vec{r}, v, t-\frac{r}{v}\right) \Phi\left(\vec{r}, v, t-\frac{r}{v}\right) \frac{\cos \theta d S_{z}}{4 \pi r^{2}}$
Only neutrons that have traveled distance $r$ without collision reach the origin. Hence, the number of neutrons scattered in direction $\vec{\Omega}$ is multiplied by the

Fig. 10.2 Contribution of point $\vec{r}$ to the flux at origin

non-interaction probability between 0 and $r$, i.e. (Glasstone and Edlund 1972, p93; Bekurts and Wirtz 1964, p104; GA tome 1 1967, p171; Planchard 1995, p5):

$$
\begin{equation*}
\text { Non-interaction probability: } \quad e^{-\int_{\ell=0}^{\ell=r} \Sigma_{l}\left(\ell, v, t-\frac{r-\ell}{v}\right) d \ell} \tag{10.1}
\end{equation*}
$$

with $\Sigma_{t}(\ell, v, t)$ the total macroscopic cross section of the medium at the current point $\vec{\ell}$.

The initial hypotheses set up assume that the total and scattering cross sections, as well as the flux, depend weakly on time and space. Hence, the phase difference in time due to $t-r / v$ can be neglected. This phase difference occurs as the current at time $t$ is the sum of the contributions from the collisions that took place earlier.

$$
\left\{\begin{array}{l}
\quad-\int_{\ell=0}^{\ell=r} \Sigma_{t}\left(\ell, v, t-\frac{r-\ell}{v}\right) d \ell \quad-\int_{\ell=0}^{\ell=r} \Sigma_{t}(\ell, v) d \ell \\
e^{\ell=0} \\
\Sigma_{s}\left(\vec{r}, v, t-\frac{r}{v}\right) \Phi\left(\vec{r}, v, t-\frac{r}{v}\right) \quad \frac{\cos \theta d S_{z}}{4 \pi r^{2}} \approx \Sigma_{s}(\vec{r}, v) \Phi(\vec{r}, v) \quad \frac{\cos \theta d S_{z}}{4 \pi r^{2}}
\end{array}\right.
$$

If the total cross section does not vary much with the space variable, $e^{-\int_{\ell=0}^{\ell=r} \Sigma_{t}(\ell, v) d \ell}$ can be simplified as $e^{-\Sigma_{t} r}$. In this case, the integration needs only to be done over the positive hemisphere $z>0$ using a spherical volume element $d^{3} r=r^{2} \sin \theta d r d \theta$ $d \varphi$ to compute the current of neutrons passing from the upper hemisphere $(z>0)$ to the lower hemisphere $(z<0), J_{z}^{-}$:

$$
J_{z}^{-} d S_{z}=\frac{\Sigma_{s}(r=0, v) d S_{z}}{4 \pi} \int_{\varphi=0}^{2 \pi} \int_{\theta=0}^{\pi / 2} \int_{r=0}^{\infty} \frac{e^{-\Sigma_{t} r} \cos \theta}{r^{2}} \Phi(\vec{r}, v) r^{2} \sin \theta d r d \theta d \varphi
$$

The scattering cross section was removed from the integral sign by assuming that its variation in space is very small. The last hypothesis (slow variation of $\Phi(\vec{r}, v)$ in space) is used to substitute the function by its first-order Taylor expansion in space:
$\Phi(\vec{r}, v)=\Phi(x, y, z, v) \approx \Phi(0,0,0, v)+x \frac{\partial \Phi}{\partial x}(0,0,0, v)+y \frac{\partial \Phi}{\partial y}(0,0,0, v)+z \frac{\partial \Phi}{\partial z}(0,0,0, v)$
This expression is inserted in the integral defining $J_{z}^{-}$, for a unit area $d S_{z}$, and by substituting $x, y, z$ by $r \sin \theta \cos \varphi, r \sin \theta \sin \varphi$ and $r \cos \theta$, with only the terms in $\Phi(0,0,0, v)$ and $\partial \Phi(0,0,0, v) / \partial z$ having a non-zero contribution:
$J_{z}^{-}=\frac{\Sigma_{s}}{4 \pi} \int_{\varphi=0}^{2 \pi} \int_{\theta=0}^{\pi / 2} \int_{r=0}^{+\infty} e^{-\Sigma_{l} r}\left[\Phi(0,0,0)+r \cos \theta \frac{\partial \Phi}{\partial z}(0,0,0)\right] \sin \theta \cos \theta d r d \theta d \varphi$
The integral over $r$ has an infinite upper bound but in practice, due to the term $e^{-\Sigma_{t} r}$, it is sufficient to integrate over a few mean free paths, i.e. $\lambda_{t}=1 / \Sigma_{t}$. Using $\Phi_{0}=\Phi(0,0,0, v)$, for the negative current, the following expression is obtained:

$$
J_{z}^{-}=\frac{\Sigma_{s}}{4 \pi} \Phi_{0} \underbrace{\int_{\varphi=0}^{2 \pi} d \varphi}_{2 \pi} \underbrace{\int_{\theta=0}^{\pi / 2} \frac{\sin 2 \theta}{2} d \theta}_{\frac{2}{4}} \underbrace{\int_{r=0}^{+\infty} e^{-\Sigma_{r} r} d r}_{\frac{1}{\Sigma_{t}}}+\frac{\Sigma_{s}}{4 \pi}\left(\frac{\partial \Phi}{\partial z}\right)_{0} \underbrace{\int_{\varphi=0}^{2 \pi} d \varphi}_{2 \pi} \underbrace{\int_{\theta=0}^{\pi / 2} \sin \theta \cos ^{2} \theta d \theta}_{\frac{1}{3}} \underbrace{\int_{r=0}^{+\infty} r e^{-\Sigma_{t} r} d r}_{\frac{1}{\Sigma_{t}^{2}}}
$$

Thence, after simplifying: $\quad J_{z}^{-}=\frac{\Sigma_{s}}{\Sigma_{t}} \frac{\Phi_{0}}{4}+\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}$
Similarly, for the positive current in the opposite direction, the following equation is obtained with a change of sign due to the integration over the lower hemisphere:

$$
J_{z}^{+}=\frac{\Sigma_{s}}{4 \pi} e^{-\Sigma_{T} r} \int_{\varphi=0}^{2 \pi} \int_{\theta=\pi / 2}^{\pi} \int_{r=0}^{+\infty}\left[\Phi_{0}+r \cos \theta\left(\frac{\partial \Phi}{\partial z}\right)_{0}\right] \sin \theta|\cos \theta| d r d \theta d \varphi
$$

Thus: $\quad J_{z}^{+}=\frac{\Sigma_{s}}{\Sigma_{t}} \frac{\Phi_{0}}{4}-\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}$
and for the net current, the balance of the positive and negative currents:

$$
J_{z}=J_{z}^{+}-J_{z}^{-}=-\frac{\Sigma_{s}}{3 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}
$$

In order to calculate $J_{x}$ and $J_{y}, z$ can be substituted successively by $x$ and $y$. The current vector is then expressed as:

$$
\vec{J}=-\frac{\Sigma_{s}}{3 \Sigma_{t}^{2}} \overrightarrow{g r a d} \Phi
$$

The proportionality coefficient between the current and the gradient is called the diffusion coefficient and has the same dimensions as a length and is often expressed in cm :

$$
\begin{equation*}
\text { Diffusion coefficient: } \quad D \equiv \frac{\Sigma_{s}}{3 \Sigma_{t}^{2}} \tag{10.2}
\end{equation*}
$$

If the flux is constant in space $\left(=\Phi_{0}\right)$, the net current is zero, which does not imply that no neutrons travel through a given surface. Using the example illustrated earlier, with the surface element $d S_{z}, \Phi_{0} / 4$ neutrons travel through the surface from the top and the same amount from the bottom, i.e. in total, $\Phi_{0} / 2$ neutrons passed through the surface per unit time (and not $\Phi_{0}$ as might wrongly be assumed! In this example, it is clear that the flux is a notion dealing with volumes and not surfaces). The net current represents the balance between these two components. If it is assumed that absorption is insignificant compared to diffusion-as is the case for well-moderated media like water reactors-this equation can be simplified since $\Sigma_{t} \approx \Sigma_{s}$, as $\Sigma_{a} \ll \Sigma_{s}$ :

Diffusion coefficient in a weakly-absorbing medium: $\quad D \approx \frac{1}{3 \Sigma_{t}}$
Fick's law, which expresses proportionality between the current and the flux gradient, is written as:

$$
\begin{equation*}
\text { Fick's law: } \quad \vec{J}=-D \overrightarrow{\operatorname{grad}} \Phi \tag{10.4}
\end{equation*}
$$

The diffusion coefficient is worth about 1 cm for conventional media employed in industrial reactors.

With these definitions, a neutron balance over a volume element implies that the time variation of the neutron population is equal to the neutron source from which absorption of neutrons is subtracted, and a leakage correction is applied at the boundaries of the volume element, i.e.:

$$
\begin{aligned}
\frac{\partial n(\vec{r}, t)}{\partial t} \equiv \frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t} & =S(t)-\Sigma_{a} \Phi(\vec{r}, t)-\operatorname{div} \vec{J}(\vec{r}, t) \\
& =S(t)-\Sigma_{a} \Phi(\vec{r}, t)+D \Delta \Phi(\vec{r}, t)
\end{aligned}
$$

### 10.1.2 Discussion of the Hypotheses

Flux, scattering and total cross sections vary slowly with time: this hypothesis is necessary to synchronize the calculation of the current with that of the scattering rate in the neighboring space. If this hypothesis is not posited, this means that the integral over time accounts for scattering events that occurred in the past such that the current and the gradient of the spatial flux are no longer correlated. In a $P W R$, the mean speed of neutrons is about $2500 \mathrm{~m} / \mathrm{s}$. The mean free path is of the order of a few centimeters and travel thus lasts around $10^{-4} \mathrm{~s}$, a duration far smaller than the time steps used for kinetic calculations in neutron physics. Hence, this hypothesis is verified for thermal reactors, which is not completely the case for fast reactors. This quasi-permanent hypothesis is to be compared to point kinetics (point reactor
model) where it is assumed that the flux may be factorized on a space function that fits the fundamental mode and depends weakly on time, and a second function which depends solely on time $\Phi(\vec{r}, t)=\Phi(\vec{r}) \quad e^{\omega t}$. The validity of the Fick's law approximation decreases as frequency $\omega$ increases (case of large reactivity insertion).

The physical medium is infinite: this hypothesis is required to integrate $e^{-\Sigma_{t} r}$. Nevertheless, since this term decreases exponentially with $r$, it can be safely stated that Fick's law is verified far from the boundaries (i.e. at a distance greater than $3 \lambda_{t}=3 / \Sigma_{t}$; this value corresponds to a distance for which $e^{-\Sigma_{l} r}$ is less than 0.05$)$.

The physical medium is uniform: thanks to this hypothesis, the non-interaction probability of neutrons on their path $r$ (as given by Eq. 10.1) can be computed analytically (in practice, it only requires that $\Sigma_{t}$ does not vary much), and furthermore, the scattering cross section can be moved out of the space integral that computes the current.

Absence of point sources of neutrons: as for the boundaries, Fick's law is verified far from sources (distance greater than $3 \lambda_{t}$ ). If sources are added, the following term must be taken into account in the space integration:

$$
S\left(\vec{r}, v, t-\frac{r}{v}\right) \frac{\cos \theta d S_{z}}{4 \pi r^{2}}
$$

It ensures that the current and the spatial flux gradient are not correlated. However, a homogeneous fission source induces the following term:

$$
\chi(v) \nu \Sigma_{f}(\vec{r}, v, t-r / v) \Phi(\vec{r}, v, t-r / v) \frac{\cos \theta d S_{z}}{4 \pi r^{2}}
$$

which, under the same simplifying hypotheses as the scattering cross section, leads to:

$$
\vec{J}(v)=-\frac{\Sigma_{s}(v)+\chi(v) \nu \Sigma_{f}(v)}{3 \Sigma_{t}^{2}} \overrightarrow{\operatorname{grad}} \Phi(v)
$$

It should be noted that in the thermal zone (and even below 20 keV ), $\chi(v)=0$. Therefore:

$$
\vec{J}=-\frac{\Sigma_{s}}{3 \Sigma_{t}^{2}} \overrightarrow{g r a d} \Phi
$$

In the fast zone of a $P W R$ where $\chi(v)=1$ and $\nu \Sigma_{f}<\Sigma_{a} \ll \Sigma_{s}$, the $\nu \Sigma_{f}+\Sigma_{s} \approx \Sigma_{t}$, approximation is warranted.

Isotropic scattering (in the laboratory frame of reference): this is the case for neutrons with low kinetic energy, with scattering anisotropy being prevalent at high energy. It should be pointed out that water has high anisotropy even for high energy.

Flux varies slowly with space: the terms in the second-order expansion of flux $\Phi(\vec{r})$ lead to an additional identical term in $J^{+}$and $J^{-}$. This term is proportional to the second derivative of flux with respect to $z$ and cancels out in the net current $J$. In fact, Fick's law $\vec{J}=-D \overrightarrow{\text { grad }} \Phi$ is valid if, for distances smaller than $3 \lambda_{t}$, the terms in the third-order expansion of $\Phi$ are negligible. From the hypotheses, the absorption rate is small compared to the scattering rate as $\Sigma_{a} \ll \Sigma_{s}$, and thus, $\Sigma_{s}$ is assumed equal to $\Sigma_{t}$. The diffusion coefficient $D$ is:

$$
D \approx \frac{1}{3 \Sigma_{t}}
$$

In the previous calculations, we supposed that the scattering collisions exhibited spherical symmetry (isotropic). In transport theory, this approximation is not used and collisions are taken into account with their complete anisotropic nature. The anisotropy of a collision can be quantified using the average cosine of the scattering angle $\overline{\mu_{0}}=\overline{\cos \vartheta}$. The mean scattering path $\lambda_{s}=1 / \Sigma_{s}$ is thus corrected due to anisotropy and is hence called the transport-corrected mean scattering path:

$$
\lambda_{s, t r} \equiv \frac{1}{\left(1-\overline{\mu_{0}}\right) \Sigma_{s}}
$$

To understand this transport correction, let us consider the anisotropy effect on the displacement of neutrons undergoing successive collisions from a geometrical point of view:

In the case of isotropic collisions, after travelling a mean scattering free path $\lambda_{s}$ following its emission, the neutron undergoes an isotropic collision that causes it to move in any direction with equal probability. After travelling a further path $\lambda_{s}$, it undergoes further collision with the same probability as previously, which can return it to its previous position with a probability of $1 /(4 \pi)$. On average, the distance travelled in a straight line by the neutron after its emission is $\lambda_{s}$, and the neutron moves about an equilibrium position. In the case of an anisotropic collision with a preferential direction as represented in Fig. 10.3 by the major axis of the ellipse, the neutron deviates from its emission point through successive collisions. The projection on the axis of emission of the neutron leads to the calculation of the average unidirectional path:

$$
\lambda_{s, t r}=\lambda_{s}+\lambda_{s}{\overline{\mu_{0}}}+\lambda_{s}{\overline{\mu_{0}}}^{2}+\lambda_{s}{\overline{\mu_{0}}}^{3}+\cdots=\lim _{n \rightarrow+\infty} \lambda_{s}\left(\frac{1-{\overline{\mu_{0}}}^{n+1}}{1-\overline{\mu_{0}}}\right)=\frac{\lambda_{s}}{1-\overline{\mu_{0}}}
$$

where $\overline{\mu_{0}} \leq 1$. This simple logic gives a physical meaning to the transportcorrected mean free scattering path $\lambda_{s, t r}$ which becomes the average distance by which the neutron deviates from a straight line emanating from its emission point:

$$
\lambda_{s, t r} \equiv \frac{\lambda_{s}}{1-\overline{\mu_{0}}}=\frac{1}{\left(1-\overline{\mu_{0}}\right) \Sigma_{s}}
$$



Fig. 10.3 Isotropic scattering (on the left) and forward anisotropy (on the right). Spheres and ellipses represent the probability density of the re-emission direction

The limit of this reasoning occurs if there is absorption, the absence of which would have brought the neutron back to its emission point after a certain time period. The transport-corrected scattering cross section becomes:

$$
\Sigma_{s, t r} \equiv\left(1-\overline{\mu_{0}}\right) \Sigma_{s}
$$

By adding the scattering cross section, the transport-corrected total cross section is:

$$
\Sigma_{t, t r} \equiv \Sigma_{a}+\left(1-\overline{\mu_{0}}\right) \Sigma_{s}=\Sigma_{t}-\overline{\mu_{0}} \Sigma_{s}
$$

In practice, the flux anisotropy induced by the anisotropy of collisions is accounted for by an expansion of flux on the basis of spherical harmonics:

$$
\Phi(\vec{r}, \vec{\Omega})=\sum_{n=0}^{\infty} \sum_{m=-n}^{+n} \varphi_{n}^{m}(\vec{r}) \quad Y_{n}^{m}(\vec{\Omega})
$$

If this expansion is limited to the first order (terms 0 and 1 ), the following is obtained:

$$
\Phi(\vec{r}, \vec{\Omega})=\frac{\Phi(\vec{r})}{4 \pi}+\frac{3}{4 \pi} \vec{\Omega} \cdot \vec{J}(\vec{r})
$$

with: $\left\{\begin{array}{l}\vec{J}(\vec{r})=-\frac{1}{3 \Sigma_{\text {transport }}} \overrightarrow{\operatorname{grad}} \Phi(\vec{r}) \\ \begin{array}{l}\text { corrected }\end{array} \\ \Sigma_{\text {transport }}=\Sigma_{t}-\bar{\mu}_{0} \Sigma_{s} \quad \text { et } \quad \Sigma_{t}=\Sigma_{a}+\Sigma_{s} \\ \text { corrected }\end{array}\right.$
and, where $\bar{\mu}_{0}$ is the average of the cosine of the scattering angle during a collision. Thus:

$$
D=\frac{1}{3\left(\Sigma_{t}-\bar{\mu}_{0} \Sigma_{s}\right)}=\frac{1}{3\left(\Sigma_{t}-\Sigma_{s, 1}\right)}=\frac{1}{3\left(\Sigma_{a}+\left(1-\bar{\mu}_{0}\right) \Sigma_{s}\right)}
$$

$\Sigma_{\text {transport }}=\Sigma_{t}-\bar{\mu}_{0} \Sigma_{s}$ is the transport-corrected cross section $\Sigma_{t r}$, often corrected
called the "transport cross section" for simplicity. This cross section is used to define the mean free transport path:

$$
\lambda_{t r} \equiv \frac{1}{\Sigma_{t r}}
$$

Use of the transport cross section in the expression of the diffusion coefficient thus transforms the diffusion equation to a $P_{1}$ approximation of the exact Boltzmann equation. Furthermore, in the case where the current depends on the transient time, the current $J_{z}^{-}(0,0,0, t)$ modeling can be improved by using a first-order Taylor expansion of the flux in space and time. This means that a neutron traveling through a surface $d S_{z}$ at time $t$ originates from a collision that occurred at time $t-r / v$ :

$$
\begin{aligned}
J_{z}^{-} & =\frac{\Sigma_{s}}{4 \pi} \int_{\varphi=0}^{2 \pi} \int_{\theta=0}^{\pi / 2} \int_{r=0}^{+\infty} e^{-\Sigma_{t} r} \Phi\left(x, y, z, t-\frac{r}{v}\right) d r \sin \theta \cos \theta d \theta d \varphi \\
& =\frac{\Sigma_{s}}{4 \pi} \int_{\varphi=0}^{2 \pi} \int_{\theta=0}^{\pi / 2} \int_{r=0}^{+\infty} e^{-\Sigma_{t} r}\left[\Phi(0,0,0, t)-\frac{r}{v}\left(\frac{\partial \Phi}{\partial t}\right)_{t}+r \cos \theta\left(\frac{\partial \Phi}{\partial z}\right)_{0}\right] d r \sin \theta \cos \theta d \theta d \varphi \\
& =\frac{\Sigma_{s}}{\Sigma_{t}} \frac{\Phi_{0}}{4}+\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}-\frac{\Sigma_{s}}{4 v \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial t}\right)_{t} \approx \frac{\Sigma_{s}}{\Sigma_{t}} \frac{\Phi_{0}}{4}+\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}-\frac{1}{v \Sigma_{t}}\left(\frac{\partial J_{z}^{-}}{\partial t}\right)_{t}
\end{aligned}
$$

Using reasoning similar to the stationary case for $J_{z}^{+}$, the following equation is obtained:

$$
J_{z}^{+} \approx \frac{\Sigma_{s}}{\Sigma_{t}} \frac{\Phi_{0}}{4}-\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}-\frac{1}{v \Sigma_{t}}\left(\frac{\partial J_{z}^{+}}{\partial t}\right)_{t}
$$

Hence, the net current along $\quad z: J_{n e t}^{z}=J_{z}^{+}-J_{z}^{-} \approx-\frac{\Sigma_{s}}{3 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial z}\right)_{0}-$ $\frac{1}{v \Sigma_{t}}\left(\frac{\partial\left(J_{z}^{+}-J_{z}^{-}\right)}{\partial t}\right)_{t}$

Therefore, the net current is:

$$
\vec{J}(\vec{r}, t)=-D\left[\overrightarrow{\operatorname{grad}} \Phi(\vec{r}, t)+\frac{3 \Sigma_{s}}{v \Sigma_{t}} \frac{\partial \vec{J}(\vec{r}, t)}{\partial t}\right] \text { with }: D \equiv \frac{\Sigma_{s}}{3 \Sigma_{t}^{2}}
$$

The result of (Weinberg and Wigner 1958, p233) and (Meghreblian and Holmes 1960, p352) under the usual hypothesis $\Sigma_{s} \approx \Sigma_{t}$ is obtained. Combined with the time-dependent transport equation:

$$
\frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t}+\operatorname{div} \vec{J}(\vec{r}, t)+\Sigma_{a} \Phi(\vec{r}, t)=S(t)
$$

and after substitution of $\vec{J}(\vec{r})$, we obtain the telegrapher's equation by analogy with the propagation of waves:

$$
\begin{equation*}
\frac{3 D}{v^{2}} \frac{\partial^{2} \Phi(\vec{r}, t)}{\partial t^{2}}+\frac{1}{v}\left(1+3 D \Sigma_{a}\right) \frac{\partial \Phi(\vec{r}, t)}{\partial t}=D \Delta \Phi(\vec{r}, t)-\Sigma_{a} \Phi(\vec{r}, t)+S(t)+\frac{3 D}{v} \frac{\partial S(t)}{\partial t} \tag{10.5}
\end{equation*}
$$

This equation is different from the usual time-dependent diffusion approximation:

$$
\frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t}=D \Delta \Phi(\vec{r}, t)-\Sigma_{a} \Phi(\vec{r}, t)+S(t)
$$

In fact, the telegrapher's equation is the exact approximation $P_{1}$ of the timedependent transport equation. Nevertheless, the usual equation is simpler to solve since it has no second-order time derivative.

### 10.1.3 The Diffusion Equation in a Force Field

Although the neutron is not influenced by electromagnetic forces, we may include an acceleration that modifies the Boltzmann equation and hence the diffusion equation (Akcasu et al. 1971, p37). The acceleration that can be taken into account is that due to gravity, which has a weak influence on neutrons of very small mass, and it has a lifetime of less than one second. This problem is more an academic than an industrial consideration but nevertheless remains a very interesting theoretical problem for establishing the transport equation. The variation in the neutron population of an element of absorbing and multiplying medium is:

$$
\frac{d n(\vec{r}, v, t)}{d t}+\Sigma_{t} \Phi(\vec{r}, v, t)=S(\vec{r}, v, t)
$$

where $S(\vec{r}, v, t)$ is the neutron source due to fission or slowing down to speed $v$. If the neutrons undergo acceleration $\vec{\gamma}$, their velocity changes between two collisions and the time derivative must be developed with the variable components:

$$
\begin{aligned}
\frac{d n(\vec{r}, v, t)}{d t}= & \frac{\partial n(\vec{r}, v, t)}{\partial t}+\vec{v} \cdot \overrightarrow{\operatorname{grad} n(\vec{r}, v, t)} \\
& +\frac{\partial v_{x}}{\partial t} \frac{\partial n(\vec{r}, v, t)}{\partial v_{x}}+\frac{\partial v_{y}}{\partial t} \frac{\partial n(\vec{r}, v, t)}{\partial v_{y}}+\frac{\partial v_{z}}{\partial t} \frac{\partial n(\vec{r}, v, t)}{\partial v_{z}}
\end{aligned}
$$

Defining the gradient with respect to the coordinates of velocity $\overrightarrow{g r a d}_{v}=$ $\left(\frac{\partial}{\partial v_{x}}, \frac{\partial}{\partial v_{y}}, \frac{\partial}{\partial v_{z}}\right)$, the previous equation may be summed up as:

$$
\frac{d n(\vec{r}, v, t)}{d t}=\frac{\partial n(\vec{r}, v, t)}{\partial t}+\vec{v} \cdot \overrightarrow{\operatorname{grad}} n(\vec{r}, v, t)+\vec{\gamma} \cdot \overrightarrow{\operatorname{grad}}_{v} n(\vec{r}, v, t)
$$

With similar reasoning as that used to establish the time-dependent telegrapher's equation, acceleration is introduced in the calculation of the neutron current by assuming that the latter is independent of the velocity:

$$
\vec{J}(\vec{r}, t)=-D \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, t)+\frac{1}{v^{2} \Sigma_{t}} \vec{\gamma}(\vec{r}, t)
$$

Combined with the neutron balance equation:

$$
\frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t}+\operatorname{div} \vec{J}(\vec{r}, t)+\Sigma_{a} \Phi(\vec{r}, t)=v \Sigma_{f} \Phi(\vec{r}, t)
$$

the diffusion equation with acceleration is obtained:

$$
\begin{equation*}
\frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t}=D \Delta \Phi(\vec{r}, t)-\frac{3 D}{v^{2}} \vec{\gamma}(\vec{r}, t) \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, t)-\Sigma_{a} \Phi(\vec{r}, t)+v \Sigma_{f} \Phi(\vec{r}, t) \tag{10.6}
\end{equation*}
$$

with $\operatorname{div}(\vec{\gamma}(\vec{r}, t))=0$. Akcasu et al. (1971, p38) develops the solution for a homogeneous slab reactor of thickness $a$, which is perpendicular to gravity. The $1 D$ diffusion equation is:

$$
\frac{1}{v} \frac{\partial \Phi(z, t)}{\partial t}=D \Delta \Phi(z, t)+\frac{3 D}{v^{2}} g \frac{\partial \Phi(z, t)}{\partial z}-\Sigma_{a} \Phi(z, t)+\nu \Sigma_{f} \Phi(z, t)
$$

For the stationary case, this equation is written in the canonical form:

$$
\Delta \Phi(z)+\mu \frac{d \Phi(z)}{d z}+B_{m}^{2} \Phi(z)=0 \quad \text { with } \quad \mu=\frac{3}{v^{2}} g \quad \text { and } \quad B_{m}^{2}=\frac{v \Sigma_{f}-\Sigma_{a}}{D}
$$

The eigenvectors are sought under the form: $\Phi_{n}(z)=\varphi_{n}(z) e^{-\frac{\mu z}{2}}$, and the usual Helmholtz equation is obtained:

$$
\Delta \varphi_{n}(z)+\left(B_{m}^{2}-\frac{\mu^{2}}{4}\right) \varphi_{n}(z)=0
$$

in which the eigenfunctions that cancel out at the boundaries $z=+a / 2$ and $z=-a / 2$ are $\varphi_{n}(z)=\cos (n \pi z / a)$. In the next chapters, we will see that the existence condition for a positive stationary flux, called the criticality condition, hinges on the fact that the eigenfunctions are solutions to the physical problem, i.e.:

$$
B_{m}^{2}-\frac{\mu^{2}}{4}=\frac{\pi^{2}}{a^{2}}
$$

Another problem of the same type consists in accounting for the flow of water from the primary loop of a $P W R$ (upward velocity of about $4 \mathrm{~m} / \mathrm{s}$ ) thereby dragging the neutrons by collision, and leading to an anisotropy that favors upward directions (distortion of the axial power). This weak effect "compensates" for gravity, causing the neutrons to "levitate".

### 10.2 Boundary Conditions for a Medium Surrounded by a Vacuum in Diffusion Theory

Given a multiplying medium surrounded by a vacuum, the incoming current can be calculated in diffusion theory (El-Wakil 1962, p113; Glasstone and Edlund 1972, p104; Glasstone and Sesonske 1994, p138; Ferziger and Zweifel 1966, p34):

$$
J_{0}^{-}=\frac{\Sigma_{s}}{\Sigma_{t}} \frac{\Phi_{0}}{4}+\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}}\left(\frac{\partial \Phi}{\partial x}\right)_{0}
$$

Since, by definition, no neutrons return to the medium from a vacuum, it can be deduced that the incoming current is zero, i.e.:

$$
J_{0}^{-}=0 .
$$

The extrapolation distance is defined as the length $d$ corresponding to the extrapolated flux according to its derivative at the medium/vacuum interface. It is given by (Fig. 10.4):

$$
\left(\frac{d \Phi}{d x}\right)_{0 \text { left }}=-\frac{\Phi_{0}}{d}<0
$$

When inserted in the equation for the current, it is equivalent to:

Fig. 10.4 Extrapolation distance of the reactor placed in a vacuum


$$
\frac{\Sigma_{s} \Phi_{0}}{4 \Sigma_{t}}-\frac{\Sigma_{s}}{6 \Sigma_{t}^{2}} \frac{\Phi_{0}}{d}=0
$$

That is:

$$
\begin{equation*}
\text { Extrapolation distance in a vacuum: } \quad d=\frac{2}{3 \Sigma_{t}}=2 D \tag{10.7}
\end{equation*}
$$

The extrapolation distance is often used to avoid meshing the reflectors in core calculations. The term zero-flux distance is sometimes used for the extrapolation distance. It should be noted that the true flux value is not zero at any point. Furthermore, it should also be pointed out that if there were a non-zero flux in vacuum, it would not be possible to represent it by the diffusion equation without a diffusion coefficient or any cross section. Only the flux in transport theory has a physical meaning. In a $l D$ medium and with simple ideas, it can be shown that transport flux is constant in a vacuum. The extrapolation distance depends solely on the diffusion coefficient of the multiplying medium. The result can be improved significantly if the value predicted by transport theory, $d=0.7104 / \Sigma_{t r}$, is used as the extrapolation distance, as noted with Milne's problem.

### 10.2.1 $\mathrm{P}_{1}$ Approximation

As seen earlier, the incoming current from a vacuum is zero and is given by:

$$
0=J_{0}^{-}=\frac{\Phi}{4}+\frac{D_{1}}{2} \overrightarrow{g r a d} \Phi
$$

The outgoing current is obtained by:

$$
J_{0}^{+}=\frac{\Phi}{4}-\frac{D_{1}}{2} \overrightarrow{\operatorname{grad}} \Phi
$$

For one dimension ( $\overrightarrow{\operatorname{grad}} \Phi=\partial \Phi / \partial x$ ), the logarithmic derivative of the flux at the interface can be computed to obtain Marshak's condition:

$$
\frac{\left(\frac{d \Phi(x)}{d x}\right)_{0^{-}}}{\Phi(0)}=-\frac{1}{2 D_{1}}=\frac{1}{\frac{2}{3} \frac{1}{\Sigma_{t}}}=-\frac{1}{\frac{2}{3} \lambda_{t}} \approx-\frac{1}{0.6667 \lambda_{t}}
$$

where $\lambda_{t}$ is the total average mean free path. If the transport-corrected $\left(\Sigma_{a}+\left(1-\bar{\mu}_{0}\right) \Sigma_{s}\right)$ mean free path $\lambda_{t r}$ is used, this is equivalent to using the $P_{1}$ transport approximation. The coefficient in the formula is corrected according to Milne's condition:

$$
\frac{\frac{d \Phi(x)}{d x}}{\Phi_{0}} \approx-\frac{1}{0.7104 \lambda_{t r}}
$$

Extrapolation of the flux through its derivative intersects the $x$ axis at the Milne extrapolation distance $d=0.7104 \lambda_{t r}$. This quantity has a very important role, since any boundary condition can exist for the diffusion equation at the edges of a multiplying medium. At the extrapolation distance, the boundary condition becomes a zero-flux condition. For power reactor cases, $d$ is very small compared to the characteristic dimensions of the reactor. Hence, as a first approximation, the flux of a reactor surrounded by a vacuum becomes zero at the geometrical boundary.

### 10.2.2 Rulko's Variational Approach

Rulko et al. showed ${ }^{1}$ that it is possible to impose a Robin-type boundary condition using the method of minimizing a functional, so as to improve the precision of the $P_{1}$ approximation. Let the neutron flux in transport theory-verifying the usual integro-differential equation-with a single kinetic energy for the sake of clarity, be:

[^235]$\left\{\begin{array}{l}\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})=\int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}+\frac{q(\vec{r})}{4 \pi} \quad \vec{r} \in V \\ \Phi(\vec{r}, \vec{\Omega})=f(\vec{r}, \vec{\Omega}) \text { at the boundary } \Gamma=\partial V \text { and for incoming directions } \vec{\Omega} \cdot \vec{n}<0\end{array}\right.$
Suppose that we wish to compute a reaction rate $R(\Phi)=\frac{1}{4 \pi} \int_{V} d \vec{r} \int_{4 \pi} \sigma^{*}(\vec{r}) \Phi$ $(\vec{r}, \vec{\Omega}) d \vec{\Omega}$ where the coefficient $1 /(4 \pi)$ is only a small shortcut in the notation for the subsequent calculations. The following functional is associated with this reaction rate:

$$
\begin{aligned}
H\left(\Phi, \Phi^{*}\right)= & \frac{1}{4 \pi} \int_{V} d \vec{r} \int_{4 \pi} \sigma^{*}(\vec{r}) \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}-\int_{V} d \vec{r} \int_{4 \pi} \Phi^{*}(\vec{r}, \vec{\Omega}) \\
& {\left[\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})-\int_{4 \pi} \Sigma_{s}(\vec{r}, \vec{\Omega}, \vec{\Omega}) \Phi(\vec{r}, \vec{\Omega}) d \vec{\Omega}-\frac{q(\vec{r})}{4 \pi}\right] d \vec{\Omega} } \\
& +\int_{\Gamma} d \vec{S} \int_{\vec{\Omega} \cdot \vec{n}<0} \vec{\Omega} \cdot \vec{n}\left(\Phi^{*}(\vec{r}, \vec{\Omega})+\alpha \Phi^{*}(\vec{r},-\vec{\Omega})\right)(\Phi(\vec{r}, \vec{\Omega})-f(\vec{r}, \vec{\Omega})) d \vec{\Omega}
\end{aligned}
$$

In this equation, $\alpha$ is a degree of freedom that will be used later and $\Phi^{*}(\vec{r}, \vec{\Omega})$ is the adjoint flux that becomes zero at the boundary of the domain and satisfies the adjoint transport equation ${ }^{2}$ with an adjoint source $\sigma^{*}(\vec{r}) /(4 \pi)$ :
$\left\{\begin{array}{l}-\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}(\vec{r}, \vec{\Omega})+\Phi^{*}(\vec{r}, \vec{\Omega}) \Sigma_{t}(\vec{r})=\int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) \Phi^{*}\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}+\frac{\sigma^{*}(\vec{r})}{4 \pi} \quad \vec{r} \in V \\ \Phi^{*}(\vec{r}, \vec{\Omega})=0 \text { at the boundary } \Gamma=\partial V \text { and for outcoming directions } \vec{\Omega} \cdot \vec{n}>0\end{array}\right.$
It can be noticed that the functional $H\left(\Phi, \Phi^{*}\right)$ is strictly equal to the required reaction rate $R(\Phi)$ using the simple properties of $\Phi(\vec{r}, \vec{\Omega})$. The latter cancels the last two integral terms for any value of $\Phi^{*}(\vec{r}, \vec{\Omega})$ and independently of that of $\alpha$. The construction of the functional $H\left(\Phi, \Phi^{*}\right)$ stems from a first-order perturbation theory. In $H$, if $\Phi$ is substituted by $\Phi+\delta \Phi$ and $\Phi^{*}$ by $\Phi^{*}+\delta \Phi^{*}$, the following expression is obtained for the first-order perturbation:

[^236]\[

$$
\begin{aligned}
& \delta H\left(\Phi, \delta \Phi, \Phi^{*}, \delta \Phi^{*}\right)= \\
& \quad-\int_{V} d \vec{r} \int_{4 \pi} \delta \Phi^{*}\left[\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi(\vec{r}, \vec{\Omega})+\Sigma_{t}(\vec{r}) \Phi(\vec{r}, \vec{\Omega})-\int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}-\frac{q(\vec{r})}{4 \pi}\right] d \vec{\Omega} \\
& -\int_{\Gamma} d \vec{S} \int_{\vec{\Omega} \cdot \vec{n}<0}|\vec{\Omega} \cdot \vec{n}|\left(\delta \Phi^{*}(\vec{r}, \vec{\Omega})+\alpha \delta \Phi^{*}(\vec{r},-\vec{\Omega})\right)(\Phi(\vec{r}, \vec{\Omega})-f(\vec{r}, \vec{\Omega})) d \vec{\Omega} \\
& -\int_{V}^{V} d \vec{r} \int_{4 \pi} \delta \Phi\left[-\vec{\Omega} \cdot \overrightarrow{g r a d} \Phi^{*}(\vec{r}, \vec{\Omega})+\Phi^{*}(\vec{r}, \vec{\Omega}) \Sigma_{t}(\vec{r})-\int_{4 \pi} \Sigma_{s}\left(\vec{r}, \vec{\Omega}, \vec{\Omega}^{\prime}\right) \Phi\left(\vec{r}, \vec{\Omega}^{\prime}\right) d \vec{\Omega}^{\prime}-\frac{\sigma^{*}(\vec{r})}{4 \pi}\right] \\
& \quad-\int_{\Gamma} d \vec{S} \int_{\vec{\Omega} \cdot \vec{n}>0} \vec{\Omega} \cdot \vec{n}\left(\delta \Phi(\vec{r}, \vec{\Omega})+\alpha \delta \Phi^{*}(\vec{r},-\vec{\Omega})\right) d \vec{\Omega}
\end{aligned}
$$
\]

An analysis of these four integral terms shows that the first and second terms cancel out each other owing to the properties of $\Phi(\vec{r}, \vec{\Omega})$ and that the last two cancel out thanks to the properties of $\Phi^{*}(\vec{r}, \vec{\Omega})$. This means that the functional $R(\Phi)$ is approximated at order two:

$$
H\left(\Phi+\delta \Phi, \Phi^{*}+\delta \Phi^{*}\right)=R(\Phi)+O\left(\delta^{2} \Phi, \delta^{2} \Phi^{*}, \delta \Phi \delta \Phi^{*}\right)
$$

Using the $P_{1}$ approximation of the flux and its adjoint, we have:

$$
\left\{\begin{array}{l}
\Phi(\vec{r}, \vec{\Omega})=\frac{1}{4 \pi}(\Phi(\vec{r})+3 \vec{\Omega} . \vec{J}(\vec{r})) \\
\Phi^{*}(\vec{r}, \vec{\Omega})=\frac{1}{4 \pi}\left(\Phi^{*}(\vec{r})+3 \vec{\Omega} \cdot \vec{J}^{*}(\vec{r})\right)
\end{array}\right.
$$

These flux expressions satisfy the selected direct and adjoint transport equations, i.e.:

$$
\left\{\begin{array}{lc}
\operatorname{div} \vec{J}+\left(\Sigma_{t}-\Sigma_{s, 0}\right) \Phi=q & -\operatorname{div} \vec{J}^{*}+\left(\Sigma_{t}-\Sigma_{s, 0}\right) \Phi^{*}=\sigma^{*} \\
\frac{1}{3} \overrightarrow{\operatorname{grad}} \Phi+\left(\Sigma_{t}-\Sigma_{s, 1}\right) \vec{J}=0 & -\frac{1}{3} \overrightarrow{\operatorname{grad}} \Phi^{*}+\vec{J}^{*}\left(\Sigma_{t}-\Sigma_{s, 1}\right)=0
\end{array}\right.
$$

Since the integral terms over volumes cancel out naturally in $\delta H\left(\Phi, \delta \Phi, \Phi^{*}, \delta \Phi^{*}\right)$, only surface integral terms remain, giving the following equation:

$$
\delta \vec{J}=-\frac{1}{3\left(\Sigma_{t}-\Sigma_{s, 1}\right)} \overrightarrow{\operatorname{grad}} \delta \Phi=-D \overrightarrow{\operatorname{grad}} \delta \Phi \text { and } \delta \vec{J}^{*}=-\left(\overrightarrow{\operatorname{grad}} \delta \Phi^{*}\right) D
$$

$$
\begin{aligned}
& \delta H\left(\Phi, \delta \Phi, \Phi^{*}, \delta \Phi^{*}\right)= \\
& -\frac{1}{4 \pi} \int_{\Gamma} d \vec{S} \int_{\vec{\Omega} \cdot \vec{n}<0} d \vec{\Omega}|\vec{\Omega} \cdot \vec{n}|\left[(1+\alpha) \delta \Phi^{*}+3(1-\alpha)\left(\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi^{*}\right) D\right] \\
& \quad \times\left[\frac{1}{4 \pi} \Phi(\vec{r}, \vec{\Omega})-\frac{3 D}{4 \pi} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi-f\right] \\
& -\frac{1}{16 \pi^{2}} \int_{\Gamma} d \vec{S} \int_{\vec{\Omega} \cdot \vec{n}>0} \vec{\Omega} \cdot \vec{n}\left(\left[\Phi^{*}+3\left(\vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}\right) D\right][(1+\alpha) \delta \Phi-3(1-\alpha) D \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi]\right) d \vec{\Omega}
\end{aligned}
$$

Rulko points out that in order to cancel out $\delta H$ at this point for any value of $\Phi, \Phi^{*}, \overrightarrow{\operatorname{grad}} \delta \Phi$ and $\overrightarrow{\operatorname{grad}} \delta \Phi^{*}$, we may artificially set up too many boundary conditions which then constrain the system. Hence, the solutions sought are such that they satisfy the Robin boundary conditions at surface $\Gamma$ :

$$
\begin{cases}\Phi+3 \lambda D \vec{n} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi=C s t & \delta \Phi=-3 \lambda D \vec{n} \cdot \overrightarrow{g r a d} \delta \Phi \\ \Phi^{*}+3 \lambda\left(\vec{n} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi^{*}\right) D=0 & \delta \Phi^{*}=-3 \lambda\left(\vec{n} \cdot \overrightarrow{\operatorname{grad}} \delta \Phi^{*}\right) D\end{cases}
$$

With this new constraint, $\delta H$ is cancelled by assuming the geometry to be a pseudo-slab geometry ( $\vec{\Omega} . \vec{n} \approx \mu$ ) such that the terms obtained from differentiation along the axes other than the major axis may be neglected at order $O\left(\delta^{2}\right)$. Hence, after some mathematical calculations:

$$
\begin{aligned}
& \delta H\left(\Phi, \delta \Phi, \Phi^{*}, \delta \Phi^{*}\right)= \\
& \quad-\frac{1}{4 \pi} \int_{\Gamma} d \vec{S} \int_{\mu=-1}^{\mu=-1} d \vec{\Omega}|\mu|\left(1-\frac{\mu}{\lambda} \frac{1-\alpha}{1+\alpha}\right) \delta \Phi^{*}\left[\frac{1}{4 \pi} \Phi-\frac{3 D}{4 \pi} \mu \vec{n} \cdot \overrightarrow{\operatorname{grad}} \Phi-f\right] \\
& \quad-\frac{1}{16 \pi^{2}} \int_{\Gamma} d \vec{S} \int_{\mu=0} \mu\left[\Phi^{*}+3 \mu \vec{n} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*} D\right] \delta \Phi\left(1+\frac{\mu}{\lambda} \frac{1-\alpha}{1+\alpha}\right) d \vec{\Omega}
\end{aligned}
$$

To cancel $\delta H$ systematically, we look for the solution that can cancel out the integrals simultaneously, i.e. after analytical integration over $\mu$ :

$$
\left\{\begin{array}{l}
\left(\frac{1}{2}+\frac{3}{\lambda} \frac{1-\alpha}{1+\alpha}\right) \Phi+\left(1+\frac{3}{4 \lambda} \frac{1-\alpha}{1+\alpha}\right) D \vec{n} \cdot \overrightarrow{\operatorname{grad}} \Phi=2 \int_{\mu=-1}^{\mu=0} d \vec{\Omega}|\mu|\left(1+\frac{|\mu|}{\lambda} \frac{1-\alpha}{1+\alpha}\right) f \\
\left(\frac{1}{2}+\frac{3}{\lambda} \frac{1-\alpha}{1+\alpha}\right) \Phi^{*}+\left(1+\frac{3}{4 \lambda} \frac{1-\alpha}{1+\alpha}\right)\left(\vec{n} \cdot \overrightarrow{\operatorname{grad}} \Phi^{*}\right) D=0
\end{array}\right.
$$

Compatibility with the Robin boundary conditions imposes the following:
$3 \lambda=\frac{\left(1+\frac{3}{4 \lambda} \frac{1-\alpha}{1+\alpha}\right)}{\left(\frac{1}{2}+\frac{3}{\lambda} \frac{1-\alpha}{1+\alpha}\right)} \quad$ and $\quad C s t e=\frac{2}{\left(\frac{1}{2}+\frac{3}{\lambda} \frac{1-\alpha}{1+\alpha}\right)} \int_{\mu=-1}^{\mu=0} d \vec{\Omega}|\mu|\left(1+\frac{|\mu|}{\lambda} \frac{1-\alpha}{1+\alpha}\right)$
From which the positive root of the first equation of second degree is obtained:

$$
\lambda=\frac{1}{1+\alpha}\left(\frac{2 \alpha}{3}+\sqrt{\frac{1}{2}-\frac{\alpha^{2}}{18}}\right)
$$

For $\alpha=1$, i.e. $\lambda=2 / 3$, the Marshak condition is obtained in its variational form:

$$
\Phi+2 D \vec{n} \cdot \overrightarrow{g r a d} \Phi=4 \int_{\mu=-1}^{\mu=0} d \vec{\Omega}|\mu| f
$$

For $\alpha=-0.0815$, i.e. $\lambda=0.7104$, we obtain the Milne condition discussed in the chapter on the Boltzmann equation. Thanks to this original approach, Rulko et al. showed through calculations that the constant value tends towards 0.750 in a heuristic manner with increasing dimensions of the $1 D$ patterns, whether slab, sphere, or cylinder. This maybe suggests a more general unified theory.

### 10.3 Boundary Conditions Between Any Two Media

In the case of two media that are in contact, diffusion theory supposes the net current to be continuous at the interface between the two media (Fig. 10.5).

The incoming current in one direction is equal to the outgoing current from the other. $\vec{J}$ is continuous and, hence, so is the flux. The law of the flux continuity implies that the outgoing current from medium 1 is equal to the incoming current for medium 2:

$$
J_{1}^{+}=J_{2}^{-}
$$

Thus:

$$
-D_{1} \overrightarrow{\operatorname{grad}} \Phi_{1} \cdot \vec{x}=-D_{2} \overrightarrow{\operatorname{grad}} \Phi_{2} \cdot \vec{x}
$$

Hence: $\quad D_{1}\left(\frac{\partial \Phi}{\partial x}\right)_{O^{-}}=D_{2}\left(\frac{\partial \Phi}{\partial x}\right)_{O^{+}}$
Fig. 10.5 Two media in contact


Fig. 10.6 Flux continuity and discontinuity of flux derivatives at the interface in diffusion


It can be seen in diffusion theory that flux is continuous at the interface, but not its derivative; this is not the case in exact transport theory. The gradient change at the interface in diffusion is proportional to $D_{1} / D_{2}$ (Fig. 10.6).

### 10.3.1 Notion of a Reflector Albedo

Let us consider two media separated by a surface. Medium 1 is assumed to be a multiplicative medium while medium 2 is a reflector. The albedo $\beta$ (from the Latin meaning "whiteness") of the reflector indexed 2 is the ratio of the outgoing current from 2, i.e. returning to medium $1(2 \rightarrow 1)$, to the incoming current in 2, i.e. leaving medium $1(1 \rightarrow 2)$ (Fig. 10.7).

$$
\beta=\frac{J_{-1}}{J_{+1}}=\frac{\frac{\Phi_{0}}{4}+\frac{D_{1}}{2}\left(\frac{d \Phi}{d x}\right)_{1}}{\frac{\Phi_{0}}{4}-\frac{D_{1}}{2}\left(\frac{d \Phi}{d x}\right)_{1}}=\frac{J_{+2}}{J_{-2}}=\frac{\frac{\Phi_{0}}{4}+\frac{D_{2}}{2}\left(\frac{d \Phi}{d x}\right)_{2}}{\frac{\Phi_{0}}{4}-\frac{D_{2}}{2}\left(\frac{d \Phi}{d x}\right)_{2}}
$$

Parameter $\beta$ characterizes the reflecting medium (2) when written in the form $\beta=J_{+2} / J_{-2}$, but it may also characterize medium 1 if written as: $\beta=J_{-1} / J_{+1}$. Medium 1 becomes, in a way, the "reflector" of medium 2. It may be noted that since $(d \Phi / d x)_{2}<0, \beta$ is smaller than 1 and tends towards 1 when $(d \Phi / d x)_{2}$ tends towards 0 , which is characteristic of a flat flux, i.e. a total reflection. This is known as a perfect reflector or a mirror, i.e. a theoretical situation that is never encountered with true media that are always absorbing to some degree. The logarithmic derivative of the flux is usually expressed as a function of the albedo:

$$
\frac{\left(\frac{d \Phi}{d x}\right)_{0^{-}}}{\Phi_{0}}=-\frac{1}{2 D_{2}} \frac{1-\beta}{1+\beta}
$$

This relation allows the substitution of a calculation with two media by a diffusion calculation on the first medium, by imposing a boundary condition on the logarithmic derivative of the flux. This is performed without calculating the flux in the reflector, thereby leading to savings in computation time. For power reactors, it is important to reduce the amount of leakage from the reactor, i.e. to obtain a flux as flat as possible, which is possible with an albedo close to 1 . In Table 10.1, it can

Fig. 10.7 Two media in contact


Table 10.1 Properties of some usual thermal reflectors

|  | $\rho_{\left[\mathrm{g} / \mathrm{cm}^{3}\right]}$ | $\lambda_{t r[\mathrm{~cm}]}$ | $D_{2[\mathrm{~cm}]}$ | $L_{[\mathrm{cm}]}$ | $\beta_{[-]}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\mathrm{D}_{2} \mathrm{O}$ (pure) | $1.10\left(20{ }^{\circ} \mathrm{C}\right)$ | 2.43 | 0.81 | 160 | 0.97 |
| Graphite | 1.60 | 2.57 | 0.86 | 52 | 0.94 |
| BeO (Beryllia) | 2.96 | 1.41 | 0.47 | 30 | 0.93 |
| Beryllium | 1.85 | 1.48 | 0.50 | 21 | 0.91 |
| Paraffin | 0.87 | 2.2 | 0.11 | 2.2 | 0.82 |
| $\mathrm{H}_{2} \mathrm{O}$ | $1.00\left(20^{\circ} \mathrm{C}\right)$ | 0.5 | 0.20 | 2.74 | 0.81 |

be observed that while water is the worst reflector among those illustrated, it remains the best industrial compromise since it is also used to cool the reactor.

The radial reflector of a $P W R$ is composed of successive materials with very different properties: steel of the baffle, water in the by-pass, steel of the core barrel, possibly the thermal shield that protects the reactor vessel depending on the reactor model, water in the down-comer, the steel of the vessel and its shaft, which is of concrete (Fig. 10.8).

We can consider that only the first 40 centimeters really influence the neutron properties of the reflector given that it is highly improbable for a neutron at that distance to be reflected back into the core. Nevertheless, the succession of highly absorbing material (steel) and a scattering moderator (water) leads to difficult homogenization calculation in diffusion theory with a homogeneous reflector material. Furthermore, given the geometrical complexity of the circumference of the core that includes square assemblies with a cylindrical reflector, calculation of the reflector is very sensitive to the industrial calculation scheme. It should be pointed out that for the European Pressurized Reactor ( $E P R$ ), the vessel is protected from fast neutrons-i.e. those causing most damage to the vesselusing a heavy steel baffle that encloses the periphery of the active core (instead of the by-pass in earlier designs, at the expense of the reflecting properties of the reflector).

### 10.4 Diffusion Equation in Energy

The diffusion equation is a simplification of the transport equation. Let the energyintegrated spatial flux be:


Fig. 10.8 Transverse view of a $900 M W e P W R$. An outline of the reflector of an industrial core

$$
\Phi(\vec{r})=\int_{0}^{\infty} \Phi(\vec{r}, E) d E=\int_{E_{t h}}^{E_{0}} \Phi(\vec{r}, E) d E
$$

where $E_{0}$ is the maximum fission energy and $E_{t h}$ the thermal energy. In the remainder of this chapter, the spatial dependence (in $\vec{r}$ ) of $\Phi$ will no longer be used to simplify the notation, $\Phi$ implying $\Phi(\vec{r})$. The neutron balance in steady state, valid for any energy $E$, is:

$$
\underbrace{\operatorname{div}(\vec{J}(r, E))+\Sigma_{t}(E) \Phi(\vec{r}, E)}_{\text {Loss of neutrons }}=\underbrace{S(\vec{r}, E)+\int_{E^{\prime}} \Phi\left(\vec{r}, E^{\prime}\right) \Sigma_{S}\left(E^{\prime} \rightarrow E\right) d E^{\prime}}_{\text {Production of neutrons }}
$$

The terms in this equation are:
$\operatorname{div}(J(\vec{r}, E))$ the leakage of neutrons from the reactor $(\vec{J}(r, E)=-D(E) \overrightarrow{\text { grad }}$ $\Phi(\vec{r}, E)$ in diffusion theory).
$\Sigma_{t}(E) \Phi(\vec{r}, E)$ the rate of neutrons lost at energy $E$ (either by absorption or by scattering) $\Sigma_{t}(E)=\Sigma_{a}(E)+\Sigma_{s}(E)$ and $\Sigma_{s}(E)=\int_{E^{\prime}} \Sigma_{S}\left(E \rightarrow E^{\prime}\right) d E^{\prime}$.
$S(\vec{r}, E)$ the source term at energy $E$, either by fission or from an independent source (often a point source) at energy $E$ (the source for starting-up reactors for example).
$\int_{E^{\prime}} \Phi\left(\vec{r}, E^{\prime}\right) \Sigma_{S}\left(E^{\prime} \rightarrow E\right) d E^{\prime}$ the scattering rate from energy $E^{\prime}$ towards energy $E$ (it thus represents a source at energy $E$ ).

### 10.5 One-Group Diffusion Equation

(Ferziger and Zweifel 1966, p19)
Integration of the diffusion equation in energy at continuous energy leads to:

$$
\begin{gathered}
\int_{E} \operatorname{div}\left(J(\vec{r}, E) d E+\int_{E} \Sigma_{a}(E) \Phi(\vec{r}, E) d E+\int_{E} \Sigma_{S}(E) \Phi(\vec{r}, E) d E\right. \\
=\int_{E} S(\vec{r}, E) d E+\int_{E} \int_{E^{\prime}} \Sigma_{S}\left(E^{\prime} \rightarrow E\right) \Phi\left(r, E^{\prime}\right) d E^{\prime} d E
\end{gathered}
$$

It can be seen that with a simple change of variable, namely $E$ to $E^{\prime}$ and $E^{\prime}$ to $E$, the integral of the scattering rate is written in two similar ways:

$$
\begin{gathered}
\int_{E} \Sigma_{S}(E) \Phi(\vec{r}, E) d E=\int_{E} \int_{E^{\prime}} \Sigma_{S}\left(E \rightarrow E^{\prime}\right) d E^{\prime} \Phi(\vec{r}, E) d E \\
=\int_{E^{\prime}} \int_{E} \Sigma_{S}\left(E^{\prime} \rightarrow E\right) d E \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}
\end{gathered}
$$

Thus, the scattering cross section can be introduced in the balance equation. Thus, after simplification, and supposing that the diffusion coefficient does not depend on space:

$$
\int_{E}-D(E) \Delta \Phi(\vec{r}, E) d E+\int_{E} \Sigma_{a}(\Phi) \Phi(\vec{r}, E) d E=\int_{E} S(\vec{r}, E) d E
$$

Let us consider the following definitions (called energy condensation):

$$
\left\{\begin{array}{l}
S \equiv \int_{E} S(\vec{r}, E) d E \quad \Sigma_{a} \equiv \frac{\int_{E} \Sigma_{a}(E) \Phi(\vec{r}, E) d E}{\int_{E} \Phi(\vec{r}, E) d E}=\frac{\int_{E} \Sigma_{a}(E) \Phi(\vec{r}, E) d E}{\Phi} \\
D \equiv \frac{\int_{E} D(E) \Phi(\vec{r}, E) d E}{\int_{E} \Phi(\vec{r}, E) d E}=\frac{\int_{E} D(E) \Phi(\vec{r}, E) d E}{\Phi}
\end{array}\right.
$$

The one-group [ $E_{t h}, E_{0}$ ] diffusion equation is written with these notations as follows:

$$
-D \Delta \Phi+\Sigma_{a} \Phi=S
$$

The source term $S$ is broken down into:

- Fission sources $\nu \Sigma_{f} \Phi$ that produce fast neutrons at the energy of the fission spectrum $\chi(E)$ (or for simplification $E_{0}$ ),
- Independent neutron sources such as the startup source with californium for the initial loading patterns, or the secondary sources with beryllium-antimony that are afterwards neglected.

$$
-D \Delta \Phi+\Sigma_{a} \Phi=v \Sigma_{f} \Phi
$$

The infinite-medium multiplication factor is defined as: $k_{\infty} \equiv \frac{\text { production }}{\text { absorption }}=\frac{v \Sigma_{f}}{\Sigma_{a}}$
Thus:

$$
\Delta \Phi+\frac{k_{\infty}-1}{\frac{D}{\Sigma_{a}}} \Phi=0
$$

The migration length is defined as:

$$
M_{[c m]} \equiv \sqrt{\frac{D}{\Sigma_{a}}}=\sqrt{\frac{\int_{E} D(E) \Phi(E) d E}{\int_{E} \Sigma_{a}(E) \Phi(E) d E}}
$$

The quantity $M^{2}=D / \Sigma_{a}$ in $\left[\mathrm{cm}^{2}\right]$ is called the migration area. The migration path $M$ must not be confused with the thermal diffusion length $L \equiv \sqrt{D_{t h} / \Sigma_{a_{t h}}}$. The former integrates the fact that the characteristic of the medium depends on the incident neutron energy. The second, $L$, applies only to thermal neutrons. The confusion arises from the fact that usually, the thermal flux equation is expressed in $\Phi_{t h}$, without the "th" index as will be seen later on.

Canonical diffusion equation for one-energy group: $\Delta \Phi+\frac{k_{\infty}-1}{M^{2}} \Phi=0$
This equation is written in the canonical form of a Helmholtz equation (historically an elliptic partial differential equation for stationary waves) as it can be solved by myriad mathematical methods depending on the geometrical context. Let us consider the following Helmholtz equation:

$$
\forall r \in V, \quad \Delta \Phi(r)+\lambda^{2} \quad \Phi(r)=0
$$

If domain $V$ is compact, the spectrum of the Laplace operator is a discrete set (Dowson 1978) and the eigenmodes $\Phi_{n}(r)$, which are solutions to the equation, form an infinite countable set such that:

$$
\forall r \in V, \quad \Delta \Phi_{n}(r)+\lambda_{n}^{2} \Phi_{n}(r)=0 \quad \text { with } \quad 0 \leq \lambda_{0}^{2} \leq \lambda_{1}^{2} \leq \lambda_{2}^{2} \leq \ldots
$$

This property has some interesting consequences in the numerical analysis of this problem to obtain the $k_{\text {eff }}$ value for a real geometry.

## 10.6 "Thermal Diffusion"

### 10.6.1 "Thermal" Diffusion Equation

If we focus more on thermal energy $E_{t h}$ which is of prime interest to the reactor physicist since it is here that the neutron density is highest, the diffusion equation applied at $E_{t h}$ is:

$$
\operatorname{div} \vec{J}\left(\vec{r}, E_{t h}\right)+\Sigma_{t}\left(E_{t h}\right) \Phi\left(\vec{r}, E_{t h}\right)=S\left(\vec{r}, E_{t h}\right)+\int_{E^{\prime}} \Phi\left(\vec{r}, E^{\prime}\right) \Sigma_{S}\left(E^{\prime} \rightarrow E_{t h}\right) d E^{\prime}
$$

The micro-reversibility principle is obtained from the non-equilibrium statistical physics relation, called the detailed balance. It relates the probability density $\omega(x)$ of a state $x$ to the conditional probability $P\left(x / x^{\prime}, t\right)$, and enables observation of the difference $x^{\prime}$ after a time period $t$, since the initial state $x$ is given by $\omega(x) P\left(x / x^{\prime}, t\right)$ $=\omega\left(x^{\prime}\right) P\left(x^{\prime} / x, t\right)$. This balance is used to demonstrate the Onsager reciprocal relations in thermodynamics. Applied to our problem, a thermal neutron has the same probability of losing as of gaining energy during a collision (only thermal neutrons can up-scatter to higher energies after a collision on a "vibrating" atom at thermal energy). It should be noted that this definition gives a precise idea of thermal energy, which has not been broached until now. This is implied by the fact that the scattering rate $\Sigma_{S}\left(E_{t h}\right) \Phi\left(\vec{r}, E_{t h}\right)$ is equal to $\int_{E^{\prime}} \Phi\left(\vec{r}, E^{\prime}\right) \Sigma_{S}\left(E^{\prime} \rightarrow E_{t h}\right) d E^{\prime}$.

That is, since $\Sigma_{S}\left(E_{t h}\right)=\int_{E^{\prime}} \Sigma_{S}\left(E_{t h} \rightarrow E^{\prime}\right) d E^{\prime}$, and by defining $\Phi_{t h}=\Phi\left(\vec{r}, E_{t h}\right)$ :

$$
\Sigma_{S}\left(E_{t h}\right) \Phi_{t h}=\int_{E^{\prime}} \Phi\left(\vec{r}, E^{\prime}\right) \Sigma_{S}\left(E^{\prime} \rightarrow E_{t h}\right) d E^{\prime}
$$

This equation is introduced in the diffusion equation expressed for $E_{t h}$, giving:

$$
-D_{t h} \Delta \Phi_{t h}+\Sigma_{a}\left(E_{t h}\right) \Phi_{t h}=S_{t h}
$$

with $D_{t h}=D\left(E_{t h}\right)$ and $\Sigma_{a_{t h}}=\Sigma_{a}\left(E_{t h}\right)$ :

$$
D_{t h} \Delta \Phi_{t h}-\Sigma_{a_{t h}} \Phi_{t h}+S_{t h}=0
$$

Using the thermal diffusion length:

$$
\begin{equation*}
\text { Thermal diffusion length: } \quad L_{[c m]}=\sqrt{\frac{D_{t h}}{\Sigma_{a_{t h}}}} \tag{10.9}
\end{equation*}
$$

and, given that every absorption of a thermal neutron creates $k_{\infty}$ more thermal neutrons by definition ${ }^{3}$ :

$$
S_{t h}=k_{\infty} \Sigma_{a_{t h}} \Phi_{t h}
$$

Hence, the canonical thermal diffusion equation:

$$
\begin{equation*}
\text { Thermal diffusion equation: } \quad \Delta \Phi_{t h}+\frac{k_{\infty}-1}{L^{2}} \Phi_{t h}=0 \tag{10.10}
\end{equation*}
$$

This thermal flux diffusion equation, also called the mono-kinetic equation, is strictly identical to the diffusion equation averaged over one energy group but evaluates constants $D$ and $\Sigma_{a}$ (hence $L$ ) at thermal energy. The thermal flux diffusion equation is also similar to the one-group flux equation assuming that the neutrons are mono-energetic at energy $E_{t h}$. This is why many authors refer to the thermal flux diffusion equation as the one-group theory by extension. The only difference comes from use of the following term in the equation:

$$
M=\sqrt{\frac{\int_{E} D(E) \Phi(E) d(E)}{\int_{E} \Sigma_{a}(E) \Phi(E) d E}} \quad \text { instead of } \quad L=\sqrt{\frac{D_{t h}}{\Sigma_{a_{t h}}}}
$$

In order to establish $M$, it is supposed that the flux can be separated into space and energy terms $\Phi(\vec{r}, E)=\Phi(E) \varphi(\vec{r})$. This expression naturally leads to the use of $M^{2}$ when the diffusion equation is integrated over the energy spectrum. This hypothesis is verified for a homogeneous medium far from the boundaries. ${ }^{4}$ For a true reactor, $M$ is far greater than $L$ since $M$ also takes into account the fact that the neutron slows down before scattering. On the other hand, $L$ assumes that the neutrons are at thermal energy. To reach thermal energy, a neutron must travel a distance that slows it down from fission energy (assuming that it has not been absorbed). It is possible to correct the transport equation to take account of non-leakage of the neutron using Fermi's age theory, as will be seen later.

[^237]
### 10.6.2 Interpretation of the Thermal Scattering Path

(Price et al. 1957, p168)
The thermal diffusion length is employed for didactic purposes: in the calculation of the mean square of the distance in a straight line. Let us consider a point source of neutrons at intensity $S$ neutrons/s. Let $r$ be the distance "as the crow flies" for a neutron scattering by collisions in the scattering medium until it is absorbed. The absorption rate in a volume defined by a sphere of radius $r$ and that at radius $r$ $+d r$ is (Fig. 10.9):

$$
4 \pi r^{2} d r \Phi(r) \Sigma_{a}(r)
$$

Supposing the problem to be isotropic (Diu et al. 2001, p78):

$$
\bar{x}=\bar{y}=\bar{z}=0 \quad \text { and } \quad \overline{x^{2}}=\overline{y^{2}}=\overline{z^{2}}=\frac{1}{3} \overline{r^{2}}
$$

The absorption probability in this same zone is proportional to the absorption reaction rate:

$$
P(r) d r=\frac{4 \pi r^{2} d r \Phi(r) \Sigma_{a}(r)}{S}
$$

Thus:

$$
\overline{r^{2}}=\int_{0}^{\infty} r^{2} P(r) d r=\frac{1}{S} \int_{0}^{\infty} 4 \pi r^{4} \Phi(r) \Sigma_{a}(r) d r
$$

The neutron flux for a point source is expressed as:

$$
\Phi(r)=\frac{S}{4 \pi D r} e^{-\sqrt{\frac{\Sigma a r}{D} r}}=\frac{S}{4 \pi D r} e^{-\frac{r}{L}}
$$

Assuming that $\Sigma_{a}(r)$ and $D$ are constant over space:

$$
\overline{r^{2}}=\frac{4 \pi}{S} \quad \int_{0}^{\infty} r^{3} \frac{S}{4 \pi D} e^{-\frac{r}{L}} \Sigma_{a}(r) d r=\frac{\Sigma_{a}}{D} \int_{0}^{\infty} r^{3} e^{-\frac{r}{L}} d r
$$

By successive integration by parts, we obtain:

$$
\int_{0}^{\infty} r^{3} e^{-\frac{r}{L}} d r=3 L \int_{0}^{\infty} r^{2} e^{-\frac{r}{L}} d r=6 L^{2} \int_{0}^{\infty} r e^{-\frac{r}{L}} d r=6 L^{4}
$$

therefore (Glasstone and Edlund 1972, p116; Meghreblian and Holmes 1960, p225):

Fig. 10.9 Scattering and absorbing sphere of radius $r$ (the picture is a $2 D$ projection of $3 D$ paths!)


Mean square distance in a straight line: $\overline{r^{2}}=\frac{\Sigma_{a}}{D} 6 L^{4}=6 L^{2}$
This expression imparts a geometrical meaning to $L$ in a non-leaking (infinite) medium. Up till now, $L$ has simply been the inverse of an attenuation coefficient. The mean square distance travelled in a straight line by a thermal neutron is exactly six times the thermal scattering area. This result must not be extrapolated at $\bar{r}$, the mean path value in a straight line, which is not equal to $\sqrt{6} L$, but this approximation of $\bar{r}$ gives the correct order of magnitude of the "scattering blot", and is more meaningful for the engineer. Besides, the term blot implies a two dimensional approach and is not very appropriate since the neutron has a three-dimensional motion. Nevertheless, it is quite common to say that the neutron scatters at thermal energy at a mean distance of two or three times the scattering path. Figure 10.10 illustrates the 3-D motion of 100 neutrons in slightly-absorbing hydrogen simulated by a Monte Carlo method and projected in a plane. The neutrons are emitted by an isotropic point source of 2 MeV placed at the center of space. The neutrons travel in a straight line (figure on the left) between two anisotropic collisions with hydrogen atoms until they are absorbed (the absorption position is represented in the figure on the right). The circle in the right-hand figure represents a surface of area $2 M^{2}$ that experimentally validates the theoretical calculation since it may be observed that most of these points are concentrated around that circle. A representation in two other projection planes leads to a similar result. Although the statistical population is low ( 100 neutrons!), the result is physically correct. It can also be observed that some neutrons may have unfolded paths that are very long compared to the radius of the scattering "smear".

This approach has been used to study Brownian motion where it is supposed that a particle moves freely and interacts by instantaneous collisions that scatter it randomly in any direction with uniform probability (isotropic collision in the


Fig. 10.10 Illustration of the paths of neutrons in hydrogen (infography Quentin Cardon 2009)
laboratory frame). In this simplified model, the diffusion coefficient is inversely proportional to the mean time between two collisions $\tau$ and is proportional to the mean square distance (Diu et al. 2001, p79):

$$
\begin{equation*}
\text { Diffusion coefficient for Brownian motion: } \quad D=\frac{1}{6} \frac{\overline{r^{2}}}{\tau} \tag{10.12}
\end{equation*}
$$

### 10.6.3 Deriving the Four-Factor Formula

For an infinite reactor, the diffusion equation $D_{t h} \Delta \Phi_{t h}-\Sigma_{a_{t h}} \Phi_{t h}+\nu \Sigma_{f_{t h}} \Phi_{t h}=0$ is simplified into $\Sigma_{a_{t h}} \Phi_{t h}=\nu \Sigma_{f t h} \Phi_{t h}$ since there is no leakage. Thus, it can be found that $k_{\infty} \Sigma_{a_{l h}}=\nu \Sigma_{f_{t h}}$ since for a permanent critical state ( $k_{\infty}=1$ ), the absorption $\Sigma_{a_{t h}} \Phi_{t h}$ produces $k_{\infty} \Sigma_{a_{t h}} \Phi_{t h}$ new neutrons and hence $k_{\infty} \Sigma_{a_{t h}} \Phi_{t h}=\nu \Sigma_{f_{t h}} \Phi_{t h}$. Using the definitions of $\eta=\nu \Sigma_{f_{t h}} / \Sigma_{a_{t h}}^{\text {fuel }}$ and of $f=\Sigma_{a_{t h}}^{f u e l} / \Sigma_{a_{t h}}$, and by noticing that the neutrons are all at thermal state, i.e. $\varepsilon=1$ and $p=1$, the formula $k_{\infty}=\nu \Sigma_{f_{t h}} / \Sigma_{a_{l h}}=\eta$ $\varepsilon p f$ is obtained.

### 10.7 Scattering of an Isotropic Source in a Non-Multiplying Medium

The diffusion equation is very helpful since it can be solved analytically in several simple geometrical cases. We will show most of these geometrical cases. The diffusion equation is linear with respect to the source term. If $G\left(\overrightarrow{r^{\prime}}, \vec{r}\right)$ is the flux induced at $\vec{r}$ by a unit source $\delta\left(\overrightarrow{r^{\prime}}-\vec{r}\right)$ placed at $\overrightarrow{r^{\prime}}$, it is called the Green function and verifies the equation:

$$
-D \Delta G\left(\overrightarrow{r^{\prime}}, \vec{r}\right)+\Sigma_{a} G\left(\overrightarrow{r^{\prime}}, \vec{r}\right)=\delta\left(\overrightarrow{r^{\prime}}-\vec{r}\right)
$$

In this case, the flux $\Phi(\vec{r})=\int_{\overrightarrow{r^{\prime}}} G\left(\overrightarrow{r^{\prime}}, \vec{r}\right) S\left(\overrightarrow{r^{\prime}}\right) d \overrightarrow{r^{\prime}}$ is the solution to the source diffusion equation in space:

$$
-D \Delta \Phi(\vec{r})+\Sigma_{a} \Phi(\vec{r})=S
$$

The linear nature of the sources is very useful for computing the flux solution in geometries with several sources.

### 10.7.1 Point Source in an Infinite Scattering Medium

Given an isotropic point source $S$ (in thermal neutrons ${ }^{5}$ per second) located at $r=0$, the whole space being filled with a non-multiplying ( $\Sigma_{f}=0, k_{\infty}=0$ ) scattering (D) and absorbing ( $\Sigma_{a}$ ) medium, the thermal diffusion equation in that medium is written for $r>0$ using the spherical symmetry of the problem:

$$
\Delta \Phi(r)-\frac{1}{L^{2}} \quad \Phi(r)=\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} \frac{d \Phi}{d r}\right)-\frac{1}{L^{2}} \quad \Phi(r)=0 \quad \text { with } \quad L^{2}=\frac{D}{\Sigma_{a}}
$$

The diffusion equation is not valid at $r=0$ due to the presence of the neutron source. It is also not valid very close to the source where, in a rigorous approach, the transport equation should be applied (although transport itself is not valid when "touching" the origin). The general solution of that differential equation is of the form:

$$
\Phi(r)=A \frac{e^{\frac{r}{L}}}{r}+B \frac{e^{-\frac{r}{L}}}{r}
$$

The boundary condition is expressed by a physical flux that is equal to zero at infinity, i.e. $\Phi(\infty)=0$, thereby leading to $A=0$. Besides, the boundary condition on the current-in $\left[\mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}\right]$-can also be used to relate it to the source:

$$
\lim _{r \rightarrow 0}\left(4 \pi r^{2} J(r)\right)=\lim _{r \rightarrow 0}\left(4 \pi r^{2}[-D \operatorname{grad} \Phi(r)]\right)=S
$$

For an isotropic spherical geometry, the gradient is expressed as $\operatorname{grad} \Phi(r)=$ $\partial \Phi(r) / \partial r$ and the current by:

[^238]$$
J(r)=-D \operatorname{grad} \Phi(r)=D B \frac{e^{-\frac{r}{L}}}{r^{2}}\left(1+\frac{r}{L}\right)
$$

Hence: $\lim _{r \rightarrow 0}\left(4 \pi r^{2} J(r)\right)=\lim _{r \rightarrow 0}\left(4 \pi r^{2} D B \frac{e^{-\frac{r}{L}}}{r^{2}}\left(1+\frac{r}{L}\right)\right)=4 \pi D B \quad$ thus: $B=\frac{S}{4 \pi D}$
Flux near a point source in a scattering and absorbing medium:

$$
\begin{equation*}
\Phi(r)_{\left[n / \mathrm{cm}^{2} / s\right]}=\frac{S_{[n / s \mathrm{~s}}}{4 \pi D} \frac{e^{-\frac{r}{L}}}{r} \tag{10.13}
\end{equation*}
$$

It can be seen that the flux tends to infinity when $r$ tends towards 0 but this solution is not physical as the diffusion equation is not valid too near the source. However, the transport flux also tends towards infinity since the uncollided flux, included in the total flux, is given by:

$$
\Phi_{s c}(r)=\frac{S}{4 \pi} \frac{e^{-\Sigma_{t} r}}{r^{2}}
$$

Any neutron emitted by the source is absorbed before reaching infinity, as showed by integrating the absorption rate:

$$
\int_{0}^{\infty} \Sigma_{a} \Phi(r) 4 \pi r^{2} d r=\int_{0}^{\infty} \frac{\Sigma_{a}}{D} S r e^{-\frac{r}{L}} d r=S \Gamma(2)=S
$$

Since the transport flux is larger than the diffusion flux close to the source and given that their absorption integrals are equal, it is logically lower than the diffusion flux far away. As seen earlier by analysis of the asymptotic transport flux, the latter is derived from a diffusion flux but we can see that there is an attenuation coefficient that is (slightly) greater than that for simplified diffusion. In reality, the asymptotic difference between transport and diffusion is very small.

The flux was plotted in Fig. 10.11 for a point in the plane (Oxy) of radius $\sqrt{x^{2}+y^{2}}$. This solution is similar to the Green function of the diffusion operator in spherical geometry (Fig. 10.12):

$$
G\left(\vec{r}, \overrightarrow{r^{\prime}}\right)=\frac{1}{4 \pi D} \frac{e^{\left.-\frac{\mid \vec{r}-r^{\prime}}{L} \right\rvert\,}}{\left|\vec{r}-\overrightarrow{r^{\prime}}\right|}
$$

The somewhat theoretical case of a non-absorbing medium is given by the Laplace equation:

Fig. 10.11 Point neutron source placed in an infinite scattering and absorbing medium


Fig. 10.12 Flux behavior near a point source
$\Phi$


$$
\Delta \Phi(r)=\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} \frac{d \Phi}{d r}\right)=0
$$

where $\Phi(\infty)=0$ and its solution that satisfies the condition $\lim _{r \rightarrow 0}\left(4 \pi r^{2} J(r)\right)=S$ is:

Flux near a point source for a non-absorbing medium: $\quad \Phi(r)_{\left[n / \mathrm{cm}^{2} / s\right]}=\frac{S_{[n / s]}}{4 \pi D r}$

This solution is to be compared to the flux produced by a point source in a vacuum, i.e. $\Phi(r)_{\text {vacuum }}=S /\left(4 \pi r^{2}\right)$. It shows that beyond a distance $D$, the flux in a scattering medium is smaller than the flux in a vacuum. Before $D$, the converse is true since some neutrons in the scattering medium are scattered backwards by collision and contribute to the flux. It should also be noted that the diffusion flux is not valid close to the source for a distance of $D$ centimeters. For the absorbing case, the probability $P(r)$ of the neutron being absorbed in a differential spherical element of thickness $4 \pi r^{2} d r$ is proportional to the absorption rate:

$$
P(r) d r=\alpha \Sigma_{a}(r) \Phi(r) 4 \pi r^{2} d r
$$

The proportionality coefficient is obtained by noticing that the probability of being absorbed in an infinite space should be equal to 1 :

$$
\lim _{R \rightarrow+\infty} \int_{0}^{R} P(r) d r=\int_{0}^{\infty} \alpha \Sigma_{a}(r) \frac{S}{4 \pi D r} e^{-\frac{r}{L}} 4 \pi r^{2} d r=\int_{0}^{\infty} \alpha \frac{S}{L^{2}} r e^{-\frac{r}{L}} d r=\alpha S \Gamma(2)=1
$$

Thus: $\quad \alpha=\frac{1}{S}$

Besides, for a unit source, $\Sigma_{a}(r) \Phi(r)$ is a probability density. Therefore, the probability that a neutron will be absorbed in a sphere of radius $R$ is:

$$
\int_{0}^{R} P(r) 4 \pi r^{2} d r=\int_{0}^{R} \alpha \frac{S}{L^{2}} r e^{-\frac{r}{L}} d r=\int_{0}^{R} \frac{1}{L^{2}} r e^{-\frac{r}{L}} d r=1-\left(\frac{R}{L}+1\right) e^{-\frac{R}{L}}
$$

Since the probability of leaking from the sphere $R$ is the complement in 1 of the probability of being absorbed inside it, the leakage probability is given by:

Leakage probability from an absorbing sphere: $\quad P_{\text {leakage }}(R)=\left(\frac{R}{L}+1\right) e^{-\frac{R}{L}}$

### 10.7.2 Anisotropic Point Source in Spherical Geometry

Using the conventional spherical coordinates:

$$
x=r \sin \theta \cos \varphi, \quad y=r \sin \theta \sin \varphi \quad \text { and } \quad z=r \cos \theta
$$

The Laplacian in these coordinates is written as:

$$
\Delta \Phi=\frac{\partial^{2} \Phi}{\partial r^{2}}+\frac{2}{r} \frac{\partial \Phi}{\partial r}+\frac{\sin ^{2} \theta}{r^{2}} \frac{\partial^{2} \Phi}{\partial(\cos \theta)^{2}}-\frac{2 \cos \theta}{r^{2}} \frac{\partial \Phi}{\partial(\cos \theta)}+\frac{1}{r^{2} \sin ^{2} \theta} \frac{\partial^{2} \Phi}{\partial \varphi^{2}}
$$

The diffusion equation for a point source is written as:

$$
\Delta \Phi(r, \theta, \varphi)-\frac{1}{L^{2}} \quad \Phi(r, \theta, \varphi)=S\left(x_{0}, y_{0}, z_{0}\right)
$$

where source $S\left(x_{0}, y_{0}, z_{0}\right)$ can be expanded as a linear combination of a Dirac distribution $\delta\left(x_{0}, y_{0}, z_{0}\right)$ and its spatial derivatives up to a certain order. It can easily be shown by linearity of the diffusion equation that, if $\psi$ is the solution to the diffusion equation with source, then the derivative $\chi \equiv \partial^{\alpha+\beta+\gamma} \psi / \partial^{\alpha} x \partial^{\beta} y \partial^{\gamma} z$ is the solution of:

$$
\begin{equation*}
\Delta \chi-\frac{1}{L^{2}} \chi=\frac{\partial^{\alpha+\beta+\gamma} S\left(x_{0}, y_{0}, z_{0}\right)}{\partial^{\alpha} x \partial^{\beta} y \partial^{\gamma} z} \tag{10.16}
\end{equation*}
$$

Alain Checroun ${ }^{6}$ studied the general solutions to the diffusion equation with a point source by supposing that the solution of the diffusion equation without source in a more general case can be factorized as:

$$
\Phi(r, \theta, \varphi) \equiv f(\cos \theta) g(\varphi) h(r)
$$

By introducing this definition in the diffusion equation without source, hence over the whole space except at the point source, we obtain:

$$
\begin{aligned}
& f g \frac{d^{2} h}{d r^{2}}+\frac{2}{r} f g \frac{d h}{d r}+\frac{\sin ^{2} \theta}{r^{2}} g h \frac{d^{2} f}{d(\cos \theta)^{2}}-\frac{2 \cos \theta}{r^{2}} g h \frac{d f}{d(\cos \theta)} \\
& +\frac{1}{r^{2} \sin ^{2} \theta} f h \frac{d^{2} g}{d \varphi^{2}}-\frac{1}{L^{2}} f g h=0
\end{aligned}
$$

By dividing by $\Phi \equiv f g h$ and multiplying by $r^{2} \sin ^{2} \theta$, the following equation is obtained:
$r^{2} \sin ^{2} \theta\left[\frac{\frac{d^{2} h}{d r^{2}}}{h}+\frac{2}{r} \frac{d h}{h} \frac{d r}{h}+\frac{\sin ^{2} \theta}{r^{2}} \frac{d^{2} f}{f d(\cos \theta)^{2}}-\frac{2 \cos \theta}{r^{2}} \frac{d f}{f d(\cos \theta)}-\frac{1}{L^{2}}\right]=-\frac{1}{g} \frac{d^{2} g}{d \varphi^{2}}=m^{2}$
It is clear that the LHS depends only on $r$ and $\theta$, while the RHS depends only on $\varphi$. These two terms are thus constants. First, we consider that the term $d^{2} g / d \varphi^{2}$ is negative and that:

[^239]$$
\frac{d^{2} g}{d \varphi^{2}}+m^{2} g=0
$$
the solutions of which are linear combinations of $\cos (m \varphi)$ and $\sin (m \varphi)$. These solutions are periodic in $\varphi$ and have a true physical meaning that exponential solutions would not have if the constant were negative.

The same mathematical trick leads to:

$$
r^{2} \frac{\frac{d^{2} h}{d r^{2}}}{h}+2 r^{\frac{d h}{r}}-\frac{r^{2}}{L^{2}}=\frac{m^{2}}{\sin ^{2} \theta}-\sin ^{2} \theta \frac{d^{2} f}{f d(\cos \theta)^{2}}+2 \cos \theta \frac{d f}{f d(\cos \theta)}
$$

where once again, the LHS depends only on $r$ and the RHS depends only on $\theta$. The constant will be written here under the form $n(n+1)$ as for the usual quantum notation. Hence, we obtain a system of differential equations as follows:

$$
\left\{\begin{array}{l}
\sin ^{2} \theta \frac{d^{2} f}{d(\cos \theta)^{2}}+2 \cos \theta \frac{d f}{d(\cos \theta)}+\left(n(n+1)-\frac{m^{2}}{\sin ^{2} \theta}\right) f=0 \\
\frac{d^{2} g}{d \varphi^{2}}+m^{2} g=0 \\
\frac{d^{2} h}{d r^{2}}+\frac{2}{r} \frac{d h}{d r}-\left(\frac{1}{L^{2}}+\frac{n(n+1)}{r^{2}}\right) h=0
\end{array}\right.
$$

The equation in $\theta$ is simply the general Legendre equation where $n$ is the degree and $m$ is the order. In mathematical references, it is often found in the following form (Abramowitz and Stegun 1972, p332):

$$
\left(1-z^{2}\right) \frac{d^{2} w}{d z^{2}}+2 z \frac{d w}{d z}+\left(\nu(\nu+1)-\frac{\mu^{2}}{\left(1-z^{2}\right)}\right) w=0
$$

The solution for $-1 \leq \cos \theta \leq 1$ is the associated Legendre function of the first kind $P_{n}^{m}(\mu)$ where $\mu \equiv \cos \theta$ and $0 \leq m \leq n$. The equation in $r$ is a modified spherical Bessel equation [see also (McLachlan 1948; Abramowitz and Stegun 1972, p443)] that is written as:

$$
\rho^{2} \frac{d^{2} h}{d \rho^{2}}+2 \rho \frac{d h}{d \rho}-\left(\rho^{2}+n(n+1)\right) h=0 \quad \text { with } \quad \rho \equiv \frac{r}{L}
$$

and its solutions are the modified spherical Bessel functions of the first kind:

$$
\sqrt{\frac{1}{2} \frac{\pi}{\rho}} I_{n+\frac{1}{2}}(\rho)=e^{-\frac{n \pi i}{2}} j_{n}\left(\rho e^{\frac{i \pi}{2}}\right) \quad \text { with } \quad j_{n}(z)=\sqrt{\frac{1}{2} \frac{\pi}{z}} J_{n+\frac{1}{2}}(z)
$$

of the second kind:

$$
\sqrt{\frac{1}{2} \frac{\pi}{\rho}} I_{-n-\frac{1}{2}}(\rho)=e^{\frac{3(n+1) \pi i}{2}} y_{n}\left(\rho e^{\frac{i \pi}{2}}\right) \quad \text { with } \quad y_{n}(z)=\sqrt{\frac{1}{2} \frac{\pi}{z}} Y_{n+\frac{1}{2}}(z)
$$

and of the third kind:

$$
\sqrt{\frac{1}{2} \frac{\pi}{\rho}} K_{n+\frac{1}{2}}(\rho)=\frac{1}{2} \pi(-1)^{n+1} \sqrt{\frac{1}{2} \frac{\pi}{\rho}}\left(I_{n+\frac{1}{2}}(\rho)-I_{-n-\frac{1}{2}}(\rho)\right)
$$

The solutions $\sqrt{\pi /(2 \rho)} I_{n+\frac{1}{2}}(\rho)$ and $\sqrt{\pi /(2 \rho)} I_{-n-\frac{1}{2}}(\rho)$ form a pair that is linearly independent for any value of $n$, as for the pair $\sqrt{\pi /(2 \rho)} I_{n+\frac{1}{2}}(\rho)$ and $\sqrt{\pi /(2 \rho)} K_{n+\frac{1}{2}}(\rho)$.

To conclude, the general solution to the Helmholtz equation without source and without any singularity on the axis $O z$ is written as:

$$
\begin{aligned}
& \Phi(r, \theta, \varphi)_{\text {without source }}=\sum_{n} \sum_{m \leq n}\left(\Phi_{n \text { even }}^{m} \cos (m \varphi)+\Phi_{n \text { odd }}^{m} \sin (m \varphi)\right) \\
& P_{n}^{m}(\cos \theta) \sqrt{\frac{1}{2} \frac{\pi}{\rho}} K_{n+\frac{1}{2}}(\rho)
\end{aligned}
$$

In this expression, the function $K_{n+\frac{1}{2}}(\rho)$ tends towards 0 as it is placed further and further away from the source, as opposed to the function $I_{n+\frac{1}{2}}(\rho)$, which tends towards infinity far from the source.

If $m=0$, the odd solution is zero, i.e. $\Phi_{n \text { odd }}^{m}=0$ and only the even solution is to be kept. This solution is not valid at the origin in the presence of a Dirac source. Checroun proposes an elegant approach that leads to a solution for the source problem. We have seen (Eq. 10.16) that the term:

$$
\psi_{n}^{m}=\left(\Phi_{n \text { even }}^{m} \cos (m \varphi)+\Phi_{n \text { odd }}^{m} \sin (m \varphi)\right) P_{n}^{m}(\cos \theta) \sqrt{\pi /(2 \rho)} K_{n+1 / 2}(\rho)
$$

can be expressed using the solution $\psi_{0}^{0}$ and its spatial derivatives of any order. If $s_{0}^{0}$ is the corresponding "source" for $\psi_{0}^{0}$, then the source sought will be expressed with $s_{0}^{0}$ and its spatial derivatives, with the same coefficients. The source $s_{0}^{0}$ of the function $\psi_{0}^{0}$ satisfies the following diffusion equation:

$$
\Delta \psi_{0}^{0}-\frac{1}{L^{2}} \quad \psi_{0}^{0}=s_{0}^{0}
$$

We can imagine the source as a sphere of radius $a$ with its center at the position of the source and set up a function corresponding to the solutions without a source and which will be zero inside the sphere. In this case, the desired source, which is a generalized function with the sphere as its support, is a discontinuity surface of the
function. By taking the limit when the radius tends towards 0 , the source is obtained by considering the distribution associated with the generalized function constituted by the source.

Let us consider the spatial Heaviside function $\Theta(r-a)$ that is zero inside the sphere and equal to 1 outside. The function $\psi \Theta(r-a)$, where $\psi$ is a solution to the diffusion equation without source everywhere in space except at the position of the point source itself, verifies the following equation:

$$
\Delta[\psi \Theta(r-a)]-\frac{1}{L^{2}} \psi \Theta(r-a)=S
$$

where $S$ is the generalized function with the sphere as support. Vector analysis allows computation of $\Delta[\psi \Theta(r-a)]$ :

$$
\begin{aligned}
\Delta[\psi \Theta(r-a)] & =\operatorname{div}(\overrightarrow{\operatorname{grad}}(\psi \Theta(r-a))) \\
& =\Theta(r-a) \Delta \psi+2\left(\frac{\partial \psi}{\partial r}+\frac{\psi}{r}\right) \delta(r-a)+\psi \frac{d \delta(r-a)}{d r}
\end{aligned}
$$

With the properties of $\Theta(r-a)$, the source of the function $\psi \Theta(r-a)$ is hence written as:

$$
S=2\left(\frac{\partial \psi}{\partial r}+\frac{\psi}{r}\right) \delta(r-a)+\psi \frac{d \delta(r-a)}{d r}
$$

The limit of this expression, when radius $a$ tends towards 0 for the function $\psi_{0}^{0}$, is given by:

$$
\psi_{0}^{0}(r)=\sqrt{\frac{1}{2} \frac{\pi}{\rho}} K_{\frac{1}{2}}(\rho)=\frac{\pi}{2 \rho} e^{-\rho}=\frac{L \pi}{2 r} e^{-\frac{r}{L}} \quad \frac{d \psi_{0}^{0}(r)}{d r}=-\frac{L \pi}{2} e^{-\frac{r}{L}}\left(\frac{1}{r^{2}}+\frac{1}{L r}\right)
$$

The scalar product of a space function $\Phi$ that can be derived infinitely and that decays rapidly far from the source is:

$$
\begin{aligned}
<S, \Phi> & \equiv \iiint \Phi(x, y, z)\left(2\left(\frac{\partial \psi_{0}^{0}}{\partial r}+\frac{\psi_{0}^{0}}{r}\right) \delta(r-a)+\psi_{0}^{0} \frac{d \delta(r-a)}{d r}\right) d x d y d z \\
& =\iiint \Phi(x, y, z)\left(\left(-\frac{\pi}{r} e^{-\frac{r}{L}}\right) \delta(r-a)+\frac{L \pi}{2 r} e^{-\frac{r}{L}} \frac{d \delta(r-a)}{d r}\right) d x d y d z
\end{aligned}
$$

With a Taylor expansion in the vicinity of the source of $\Phi(x, y, z)$ and for the exponential:

\[

\]

and with a volume element in spherical geometry:

$$
d v=r^{2} d r \sin \theta d \theta d \varphi
$$

Therefore:

$$
\begin{aligned}
& <S, \Phi>=\int_{r=0}^{r=+\infty} r^{2} d r \int_{\theta=0}^{\theta=\pi} \sin \theta d \theta \int_{\varphi=0}^{\varphi=2 \pi} \\
& d \varphi\left(\Phi\left(x_{0}, y_{0}, z_{0}\right)+r\left(\left.\sin \theta \cos \varphi \frac{\partial \Phi}{\partial x}\right|_{x_{0}}+\left.\sin \theta \sin \varphi \frac{\partial \Phi}{\partial y}\right|_{y_{0}}+\left.\cos \theta \frac{\partial \Phi}{\partial z}\right|_{z_{0}}\right)+\ldots\right) \\
& \quad \times\left(-\frac{2}{L} \delta(r-a)+\frac{d \delta(r-a)}{d r}\right) \frac{L \pi}{2 r}\left(1-\frac{r}{L}+\frac{1}{2}\left(\frac{r}{L}\right)^{2}-\frac{1}{6}\left(\frac{r}{L}\right)^{3}+\ldots\right)
\end{aligned}
$$

Using the following property of the Dirac distribution:

$$
<f(r), \delta(r-a)>=f(a) \quad \text { and } \quad<f(r), \frac{d \delta(r-a)}{d r}>=-\left.\frac{d f(r)}{d r}\right|_{a}
$$

Hence, all the terms of the integral that multiply $\delta(r-a)$ introduce a coefficient $a^{p}$ with $p>1$ the exponent being due to the expansion of the exponential term, and hence, tend towards 0 when $a$ tends towards 0 . For the terms that multiply $d \delta(r-a) /$ $d r$, only the constant term taken from the derivative of $r^{2} \times L \pi /(2 r)$ remains, i.e. $L \pi / 2$.

Finally, after integration, we obtain:

$$
\lim _{a \rightarrow 0}<S, \Phi>=\int_{\theta=0}^{\theta=\pi} \sin \theta d \theta \int_{\varphi=0}^{\varphi=2 \pi} d \varphi\left(-\frac{L \pi}{2} \Phi\left(x_{0}, y_{0}, z_{0}\right)\right)=-2 \pi^{2} L \Phi\left(x_{0}, y_{0}, z_{0}\right)
$$

Hence, the source corresponding to the function $\psi_{0}^{0}(r)=\sqrt{\frac{1}{2}} \frac{\pi}{\rho} K_{\frac{1}{2}}(\rho)=$ $\frac{\pi}{2 \rho} e^{-\rho}=\frac{L \pi}{2 r} e^{-\frac{r}{L}}$ is equal to

$$
S_{0}^{0}=-2 \pi^{2} L \delta\left(x-x_{0}, y-y_{0}, z-z_{0}\right)
$$

It may be noted that this source is negative as it "compensates" for the behavior of the spatial function $\sqrt{\pi /(2 \rho)} K_{1 / 2}(\rho)$ that tends rapidly towards infinity when $\rho$ tends towards 0 .

Using some very complex calculations, we can compute the derivatives of the function $\psi_{0}^{0}(r)$ with respect to $x, y$ and $z$, as well as the cross-derivatives and the $n^{\text {th }}$ derivatives. From the previous discussions, we can deduce the source $S_{n}^{m}$ of the solution $\psi_{n}^{m}$, as a function of $\delta$ and its derivatives up to the order $m+n$ with respect to $x, y$ and $z$. Calculation of the coefficients is carried out subsequently using recurrence relations adapted to computer programming. This approach is equivalent to expansion of the function $\Phi$ using a basis consisting of source functions $S_{n}^{m}$ by calculating the moments $<S_{n}^{m}, \Phi>$ successively. The angular parts in $\theta$ and $\varphi$ may be computed by if the angular distribution of the point source is known. In the chapter on "Critical pile theory", it will be seen that the previous technique can be applied to a point source in a multiplying medium.

### 10.7.3 Infinite Thin Rod Source in an Infinite Scattering Medium

Let us consider an isotropic source of thermal neutrons in the form of a thin (wirelike or line) rod $S$ (in neutrons per second and per cm of length of wire) situated at $r=0$. The whole space is filled with a non-multiplying scattering and absorbing medium. The thermal diffusion equation in the medium is written for $r>0$, using the cylindrical symmetry of the problem:

$$
\begin{gathered}
\Delta \Phi(r)+\frac{k_{\infty}-1}{L^{2}} \quad \Phi(r)=\frac{1}{r} \frac{d}{d r}\left(r \frac{d \Phi}{d r}\right)-\frac{1}{L^{2}} \Phi(r)=0 \quad \text { with } \quad L^{2}=\frac{D}{\Sigma_{a}} \\
\frac{1}{r} \frac{d}{d r}\left(r \frac{d \Phi}{d r}\right)-\frac{1}{L^{2}} \Phi(r)=\frac{d^{2} \Phi(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi(r)}{d r}-\frac{1}{L^{2}} \quad \Phi(r)=0
\end{gathered}
$$

that can be written in the form of a modified Bessel equation by multiplying by $r^{2}$ (Fig. 10.13):

$$
r^{2} \frac{d^{2} \Phi(r)}{d r^{2}}+r \frac{d \Phi(r)}{d r}-\frac{1}{L^{2}} r^{2} \Phi(r)=0
$$

The solution to such an equation may be written in the form:

$$
\Phi(r)=A I_{0}\left(\frac{r}{L}\right)+B \quad K_{0}\left(\frac{r}{L}\right)
$$

where $I_{0}$ and $K_{0}$ are modified Bessel functions of the first and second kind of order 0 . Moreover, the boundary condition on current $J$ that relates it to the source may be used:

Fig. 10.13 Wire-like neutron source placed in an infinite scattering and absorbing medium


$$
\begin{aligned}
\lim _{r \rightarrow 0}(2 \pi r J(r)) & =\lim _{r \rightarrow 0}(2 \pi r[-D\|\overrightarrow{\operatorname{grad}} \Phi(r)\|])=\lim _{r \rightarrow 0}\left(2 \pi r\left(D \frac{B}{L} K_{1}\left(\frac{r}{L}\right)\right)\right) \\
& =S_{[n / c m / s]}
\end{aligned}
$$

Using the expansion of the Bessel function in the vicinity of 0 :

$$
K_{1}(x)=\left(\gamma+\log \left(\frac{x}{2}\right)\right) I_{1}(x)+\frac{1}{x}-\frac{x}{4}+\frac{5 x^{3}}{64}+. .
$$

and that of: $\quad I_{1}(x)=\frac{x}{2}+\frac{x^{3}}{16}+\frac{x^{5}}{384}+\ldots$
we obtain: $\quad \lim _{r \rightarrow 0}(2 \pi r J(r))=\lim _{r \rightarrow 0}\left(2 \pi r D \frac{B}{L}\left[\left(\gamma+\log \left(\frac{r}{2 L}\right)\right) I_{1}\left(\frac{r}{L}\right)+\frac{L}{r}\right]\right)$

$$
=2 \pi D B=S_{[n / \mathrm{cm} / \mathrm{s}]}
$$

Hence: $B=\frac{S}{2 \pi D}$
and: Flux of a line source: $\quad \Phi(r)_{\left[n / \mathrm{cm}^{2} / \mathrm{s}\right]}=\frac{S_{[n / \mathrm{cm} / \mathrm{s}]}}{2 \pi D} K_{0}\left(\frac{r}{L}\right)$
It can be noted that as in the case of a point source, the flux tends towards infinity when $r$ tends towards 0 , and that this solution is not physical as the diffusion equation is not valid close to the source. The transport equation is not valid either if the distance being considered is smaller than the size of the neutron and the transport flux also tends towards infinity very close to the source.

### 10.7.4 Infinite Plane Source in an Infinite Scattering Medium

Let $S$ be an infinite isotropic plane source (in neutrons per second and per $\mathrm{cm}^{2}$ of source surface) located at $x=0$. The whole space is filled with a non-multiplying scattering and absorbing medium (with the characteristics $D$ and $L$ or $\kappa=1 / L$ ). The diffusion equation in the medium is written as:

$$
\Delta \Phi(x)-\frac{1}{L^{2}} \Phi(x)=\frac{d^{2} \Phi(x)}{d x^{2}}-\frac{1}{L^{2}} \quad \Phi(x)=0
$$

The solution to this differential equation is of the form (Fig. 10.14):

$$
\Phi(x)=A e^{+\frac{x}{L}}+B e^{-\frac{x}{L}}=A e^{+\kappa x}+B e^{-\kappa x}
$$

The boundary condition is expressed by $\Phi(\infty)=0$ and $\Phi(-\infty)=0$. On the right, $\Phi(\infty)=0$ leads to $A=0$. At $x=0$, the source is isotropic and induces a current of $S / 2$ on each side, therefore:


Fig. 10.14 Plane neutron source placed in an infinite scattering and absorbing medium

$$
\lim _{x \rightarrow 0}(J(x))=\lim _{x \rightarrow 0}(-D \operatorname{grad} \Phi(x))=D \frac{B}{L}=\frac{S}{2} \quad \text { hence } \quad B=\frac{S L}{2 D}
$$

$$
\text { On the right: } \quad \Phi(x)_{\left[n / \mathrm{cm}^{2} / \mathrm{s}\right]}=\frac{S_{\left[n / \mathrm{cm}^{2} / \mathrm{s}\right]}}{2} \frac{L_{[\mathrm{cm}]}}{D_{[c m]}} e^{-\frac{x}{L}}
$$

On the left, $\Phi(-\infty)=0$ leads to $B=0$, where: $\Phi(x)=A e^{\frac{x}{t}}$. The same reasoning as for the right leads to $\Phi(x)=S L e^{\frac{x}{L}} /(2 D)$. The two solutions to the symmetrical flux are given by:

$$
\begin{equation*}
\text { Flux for a plane source: } \quad \Phi(x)=\frac{S}{2} \frac{L}{D} e^{-\frac{|x|}{L}}=\frac{S}{2 \kappa D} e^{-\kappa|x|} \tag{10.18}
\end{equation*}
$$

This solution is to be compared with the flux emitted by a plane source in a vacuum. Assuming that the diffusion equation is applicable to a vacuum, when the absorption cross section tends towards 0 , the diffusion coefficient tends towards infinity as well as the migration length. Thus, the following equation is to be solved for a plane geometry:

$$
\Delta \Phi(x)=0
$$

Its general solution with source boundary conditions is:

$$
\Phi(x)=\frac{S}{2}
$$

For a real scattering medium, the probability of a neutron being absorbed in the range $d x$ is proportional to the absorption rate:

$$
P(x) d x=\alpha \Sigma_{a} \Phi(x) d x=\alpha \Sigma_{a} \frac{S}{2} \frac{L}{D} e^{-\frac{x}{L}} d x=\alpha \frac{S}{2 L} e^{-\frac{x}{L}} d x
$$

All neutrons are obviously absorbed between 0 and infinity, hence allowing a normalization condition to be sought:

$$
\int_{0}^{+\infty} P(x) d x=\alpha \frac{S}{2}=1 \Rightarrow P(x)=\frac{1}{L} e^{-\frac{x}{L}} d x
$$

The mean square distance travelled can thus be computed:

$$
\overline{x^{2}}=\int_{0}^{+\infty} x^{2} P(x) d x=L^{2} \underbrace{\int_{0}^{+\infty}\left(\frac{x}{L}\right)^{2} e^{-\frac{x}{L}} \frac{d x}{L}}_{\Gamma(3)=2}=2 L^{2}
$$

This value is to be compared for a three-dimensional path of the neutron in spherical geometry, i.e. $\overline{r^{2}}=6 L^{2}$. Given that:

$$
r^{2}=x^{2}+y^{2}+z^{2}
$$

Since $\overline{x^{2}}=\overline{y^{2}}=\overline{z^{2}}=2 L^{2}$, we obtain (Fig. 10.15)

$$
\overline{r^{2}}=\overline{x^{2}}+\overline{y^{2}}+\overline{z^{2}}=6 L^{2}
$$

### 10.7.5 Infinite Plane Source in an Infinite Scattering Slab

Let us consider another case with an isotropic infinite plane source $S$ (in neutrons per second and per $\mathrm{cm}^{2}$ of source surface) located at $x=0$, but this time, placed at the center of a scattering and absorbing infinite slab with axes $y$ and $z$. The latter is a non-multiplying medium (with properties $D$ and $L$ ). The flux is sought such that it is equal to zero at the boundaries of the scattering wall. The diffusion equation for the medium is written as for the previous case, except that this time, the boundary conditions are different. Instead of having a solution as a combination of exponential terms, for simplicity, we choose the solution in the following form (Fig. 10.16):


Fig. 10.15 Plane projection of the three-dimensional trajectory of the neutron


Fig. 10.16 Plane neutron source placed at the center of an infinite scattering and absorbing slab

$$
\Phi(x)=A \operatorname{sh}\left(\frac{x}{L}\right)+B \operatorname{ch}\left(\frac{x}{L}\right)
$$

The zero-flux boundary conditions at $x=+a / 2$ and $x=-a / 2$ are implemented as:

$$
\begin{aligned}
& \qquad A \operatorname{sh}\left(\frac{a}{2 L}\right)+B \operatorname{ch}\left(\frac{a}{2 L}\right)=0 \\
& \text { Therefore: } \quad B=-\frac{A \operatorname{sh}\left(\frac{a}{2 L}\right)}{\operatorname{ch}\left(\frac{a}{2 L}\right)}=-A \operatorname{th} \frac{a}{2 L}
\end{aligned}
$$

Assuming an isotropic source that emits $S / 2$ neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$ in the positive $x$ direction, the current at the origin is given by:

$$
-D\left(\frac{\partial \Phi(x)}{\partial x}\right)_{0}=-D\left(\frac{A}{L} \operatorname{ch}(0)+\frac{B}{L} \operatorname{sh}(0)\right)=-D \frac{A}{L}=\frac{S}{2}
$$

Thus, the constant $A$ is equal to: $A=-\frac{S L}{2 D}$
Introducing these values in the expression of the flux leads to:
$\Phi(x)=-\frac{S L}{2 D} \operatorname{sh}\left(\frac{x}{L}\right)+\frac{S L}{2 D} \frac{\operatorname{sh}\left(\frac{a}{2 L}\right)}{\operatorname{ch}\left(\frac{a}{2 L}\right)} \operatorname{ch}\left(\frac{x}{L}\right)=\frac{S L}{2 D}\left(\frac{-\operatorname{sh}\left(\frac{x}{L}\right) \operatorname{ch}\left(\frac{a}{2 L}\right)+\operatorname{sh}\left(\frac{a}{2 L}\right) \operatorname{ch}\left(\frac{x}{L}\right)}{\operatorname{ch}\left(\frac{a}{2 L}\right)}\right)$
Similar reasoning for the negative $x$ direction and a zero-flux condition at $x=-a / 2$ leads to a general solution that is valid for any scattering wall:

$$
\Phi(x)=\frac{S L}{2 D}\left(\frac{\operatorname{sh}\left(\frac{a}{2 L}-\frac{|x|}{L}\right)}{\operatorname{ch}\left(\frac{a}{2 L}\right)}\right)
$$

This equation can also be written by using the fact that $\Phi(0)=\frac{S L}{2 D} \operatorname{th}\left(\frac{a}{2 L}\right)$ :

$$
\begin{equation*}
\text { Flux for a scattering wall: } \quad \Phi(x)=\Phi(0)\left(\frac{\operatorname{sh}\left(\frac{a}{2 L}-\frac{|x|}{L}\right)}{\operatorname{sh}\left(\frac{a}{2 L}\right)}\right) \tag{10.19}
\end{equation*}
$$

### 10.7.6 Uniform Source in an Infinite Scattering Slab

This case is slightly different from the previous one since the source $S$ is now isotropic and uniformly distributed in the slab thickness (in neutrons per second and per $\mathrm{cm}^{3}$ of slab). The slab is scattering and absorbing with the same properties as in the previous case. The flux is sought using a zero-flux boundary condition at the edge of the wall (Fig. 10.17).

Fig. 10.17 Uniform neutron source in the volume


Strictly speaking, the diffusion equation should not be applied in the presence of sources as is the case here. The diffusion equation in the medium is similar to that in the previous case. Therefore, the general solution of the homogeneous differential equation is:

$$
\Phi(x)=A e^{\frac{x}{L}}+B e^{-\frac{x}{L}}
$$

or even: $\Phi(x)=A \operatorname{sh}(x / L)+B \operatorname{ch}(x / L)$. A particular solution for the inhomogeneous equation is the trivial solution that is independent of space: $\Phi(x)=L^{2}$ $S / D=S / \Sigma_{a}$. The general solution to the inhomogeneous equation is the sum of the particular solution to the inhomogeneous equation and the general solution to the homogeneous equation:

$$
\Phi(x)=A \operatorname{sh}\left(\frac{x}{L}\right)+B \operatorname{ch}\left(\frac{x}{L}\right)+\frac{S}{\Sigma_{a}}
$$

The zero-flux boundary conditions at $x=+a / 2$ induces the following equation:

$$
A \operatorname{sh}\left(\frac{a}{2 L}\right)+B \operatorname{ch}\left(\frac{a}{2 L}\right)+\frac{S}{\Sigma_{a}}=0
$$

The current is continuous and is equal to zero at the center by symmetry:

$$
-D\left(\frac{\partial \Phi(x)}{\partial x}\right)_{0}=-D\left(\frac{A}{L} \operatorname{ch}\left(\frac{0}{L}\right)+\frac{B}{L} \operatorname{sh}\left(\frac{0}{L}\right)\right)=-D \frac{A}{L}=0 \quad \text { hence: } \quad A=0
$$

The boundary conditions inserted in the flux solution lead to:

$$
\Phi(x)=\frac{S}{\Sigma_{a}}\left(1-\frac{\operatorname{ch}\left(\frac{x}{L}\right)}{\operatorname{ch}\left(\frac{a}{2 L}\right)}\right)
$$

At $x=0, \Phi(0)=\frac{S}{\Sigma_{a}}\left(1-\frac{1}{\operatorname{ch}\left(\frac{a}{2 L}\right)}\right)>0$ since $\operatorname{ch}\left(\frac{a}{2 L}\right)>1$
Unlike the previous case for the scattering of plane source in a scattering slab, the flux curvature is negative for a source uniformly distributed in the volume. This situation will also be encountered for over-critical multiplying media.

### 10.7.7 Semi-infinite Slab Source

The isotropic source $S$ is uniformly distributed in a semi-infinite slab for $x<0$ (in neutron per second and par $\mathrm{cm}^{3}$ of slab). The $x>0$ half space is scattering and
absorbing with the same properties as the left side. Flux is sought so as to have a 0 solution at the positive infinite. In this case, the previously calculated solution for a plane source will be used with the analogy of the slab as a successive pattern of planes of infinitesimal thickness $d y$ (Fig. 10.18).

Each contribution of the slice of thickness $d y$ to the flux is given by:

$$
\Phi_{y}(x)=\frac{S d y L}{2 D} e^{-\frac{x-y}{L}}
$$

$S d y$ representing a plane source at the point of negative $y$. The total flux at point $x$ is the sum of all contributions of these plane sources in $y$, assuming that the sources do not interact with one another, i.e.:

$$
\Phi(x)=\int_{y=-\infty}^{y=0} \frac{S d y L}{2 D} e^{-\frac{x-y}{L}}=\frac{S L^{2}}{2 D} e^{-\frac{x}{L}}
$$

This method may be adapted if the slab has a thickness of $y_{2}-y_{1}$ where $y_{1}$ and $y_{2}$ are positive:

$$
\Phi(x)=\int_{y=y_{1}}^{y=y_{2}} \frac{S d y L}{2 D} e^{-\frac{x-y}{L}}=\frac{S L^{2}}{2 D}\left(e^{-\frac{x-y_{2}}{L}}-e^{-\frac{x-y_{1}}{L}}\right)
$$

We obtain the solution for the semi-infinite slab by setting $y_{2}=0$ and $y_{1}=-\infty$. Hence, the method can be extended to a set of slabs with finite thickness, or even if the slab is purely absorbing.

Fig. 10.18 Semi-infinite slab source in the half plane $x<0$


### 10.7.8 Extension to the Infinite Homogeneous Medium

If we seek the solution for a flux such that it is bonded over the whole space consisting of a homogeneous absorbing non-multiplying medium and such that:

$$
-D \Delta \Phi(x)+\Sigma_{a} \Phi(x)=S(x)
$$

Given any source form, the Laplacian operator in slab geometry has the eigenfunctions $e^{-i b x}$ and $e^{+i b x}$, thereby implying the following Fourier transform:

$$
\left\{\begin{array} { l } 
{ \varphi ( b ) = \int _ { - \infty } ^ { + \infty } e ^ { i b x } \Phi ( x ) d x } \\
{ s ( b ) = \int _ { - \infty } ^ { + \infty } e ^ { i b x } S ( x ) d x }
\end{array} \left\{\begin{array}{l}
\Phi(x)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i b x} \varphi(b) d b \\
s(x)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i b x} s(b) d b
\end{array}\right.\right.
$$

When applied to the diffusion equation, the relation between the flux and the source is:

$$
\varphi(b)=\frac{s(b)}{D b^{2}+\Sigma_{a}}
$$

With the inverse transform, the following equation is obtained:

$$
\begin{gathered}
\Phi(x)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i b x} \frac{s(b)}{D b^{2}+\Sigma_{a}} d b=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i b x} \frac{\int_{-\infty}^{+\infty} e^{i b y} S(y) d y}{D b^{2}+\Sigma_{a}} d b \\
=\frac{1}{4 \pi \kappa D} \int_{-\infty}^{+\infty} d y S(y) \int_{-\infty}^{+\infty} \frac{2 \kappa}{b^{2}+\kappa^{2}} e^{-i b(x-y)} d b
\end{gathered}
$$

with $\kappa^{2}=\Sigma_{a} / D$. The Fourier transform of the function $e^{-\kappa|x|}$ is given by:

$$
\int_{-\infty}^{+\infty} e^{i b x} e^{-\kappa|x|} d x=\frac{2 \kappa}{b^{2}+\kappa^{2}} \quad \text { and } \quad \int_{-\infty}^{+\infty} e^{-i b x} \frac{2 \kappa}{b^{2}+\kappa^{2}} d b=2 \pi e^{-\kappa|x|}
$$

This is in fact the inverse transform of the flux expression. Therefore:

$$
\Phi(x)=\frac{1}{2 \kappa D} \int_{-\infty}^{+\infty} e^{-\kappa|x-y|} S(y) d y
$$

It is the convolution of the plane Green function $G\left(\vec{r}, \vec{r}^{\prime}\right)=e^{-\kappa\left|\vec{r}-\vec{r}^{\prime}\right|} /(2 \kappa D)$ with the source, thereby confirming the linear nature of the equation. This property allows calculation of the flux by summing the contributions from the various sources.

### 10.7.9 Expansion on the Eigenfunctions of the Laplacian Operator

Let us consider the case of a slab of thickness $a$ with a source $S(x)$. The flux solution is obtained with zero-flux boundary conditions at $+a / 2$ and $-a / 2$. If the source is not symmetric, it is not possible to ensure that the solution is even. The equation for diffusion in the slab is:

$$
\Delta \Phi(x)-\frac{1}{L^{2}} \Phi(x)=-\frac{S(x)}{D}
$$

The general solutions to the homogeneous equation are of the form $e^{-\frac{x}{L}}$ and $e^{+\frac{x}{L}}$, which are eigenfunctions of the Laplacian in infinite slab geometry. However, let us seek solutions in the form of decomposition on an orthogonal basis $e^{-i B x}$ and $e^{+i B x}$ (or $\sin B x$ and $\cos B x$ ), eigenfunctions in finite geometry. Since flux is zero at the boundaries, functions of the form:

$$
\Phi_{n}(x)=\varphi_{n} \cos \left(\frac{n \pi}{a} x\right) \quad n \text { odd }
$$

are solutions to the problem. The eigenfunctions of the Laplacian are orthogonal, i.e.:

$$
\int_{-\frac{a}{2}}^{+\frac{a}{2}} \Phi_{n}(x) \Phi_{m}(x) d x=\frac{a}{2} \delta_{n, m}
$$

The flux and the source are expanded on this particular basis:

$$
\Phi(x)=\sum_{k=1}^{\infty} \varphi_{k} \Phi_{k}(x) \quad \text { and } \quad S(x)=\sum_{k=1}^{\infty} s_{k} \Phi_{k}(x)
$$

and the latter are inserted in the diffusion equation that includes a source, i.e.:

$$
\sum_{k=1}^{\infty} \varphi_{k}\left(-B_{k}^{2}-\frac{1}{L^{2}}\right) \Phi_{k}(x)=-\frac{\sum_{k=1}^{\infty} s_{k} \Phi_{k}(x)}{D}
$$

The term-to-term identification of this expansion in a base of complete continuous functions on the interval $[-a / 2,+a / 2]$ leads to the flux moment of order $k$ :

$$
\varphi_{k}=\frac{s_{k}}{D\left(B_{k}^{2}+\frac{1}{L^{2}}\right)}
$$

Bearing in mind that the source moment is obtained by: $s_{k}=\frac{2}{a} \int_{-\frac{a}{2}}^{+\frac{a}{2}} \Phi_{k}(x) S(x) d x$ :

$$
\Phi(x)=\int_{-\frac{a}{2}}^{+\frac{a}{2}} \frac{2}{a} \sum_{k=1}^{\infty} \frac{\Phi_{k}(x) \Phi_{k}\left(x^{\prime}\right)}{D\left(B_{k}^{2}+\frac{1}{L^{2}}\right)} S\left(x^{\prime}\right) d x^{\prime}
$$

Duderstadt and Hamilton (1976) point out that in this way, expansion is obtained of the plane Green function with zero flux at the boundaries of the slab:

$$
G\left(x, x^{\prime}\right)=\frac{2}{a} \sum_{k=1}^{\infty} \frac{\Phi_{k}(x) \Phi_{k}\left(x^{\prime}\right)}{D\left(B_{k}^{2}+\frac{1}{L^{2}}\right)}
$$

This result can be extended to any homogeneous geometry with zero flux conditions at the surface (cylinder, sphere) by substituting $x$ coordinate by position $\vec{r}$ and by using the eigenfunctions of the Laplacian associated to the given geometry. In practice, expansion is limited to a finite order. For a problem with non-zero flux conditions at boundaries, all the eigenfunctions should be kept, especially the sine functions in the plane.

### 10.7.10 Superposition of Flux Induced by Point Sources

We have just considered the case in which the flux calculation was carried out by summing over the plane solution for a slab, and for an infinite medium. The calculation by summing is justified so long as the diffusion equation remains linear, i.e. the flux resulting from two different sources can be added if there is no interaction between the latter (e.g. sources coupled by the flux). Generally, the flux is the convolution of the Green function for the given geometry and the independently distributed sources.

This approach can be extended by considering any independent source (Fig. 10.19) as the sum of quasi-point sources for which the contributions convoluted by the spherical Green function are summed:

Fig. 10.19 Slab source of finite thickness


Fig. 10.20 Integration over point sources


$$
\Phi(\vec{r})=\int_{V} S\left(\overrightarrow{r^{\prime}}\right) \frac{e^{-\frac{\left|\vec{r}-\vec{r}^{\prime}\right|}{L}}}{4 \pi D\left|\vec{r}-\vec{r}^{\prime}\right| d^{3} r^{\prime}}
$$

For illustration (Glasstone and Edlund 1972, p110), the flux at a point on the $x$ axis can be calculated as the contribution of the point sources forming a loop of thickness $d r$ in a source plane (Fig. 10.20):
$r^{\prime 2}=r^{2}+x^{2}$ where: $r^{\prime} d r^{\prime}=r d r$

$$
\Phi(x)=\int_{r^{\prime}=x}^{r^{\prime}=+\infty} \frac{e^{-\frac{r^{\prime}}{L}}}{4 \pi D r^{\prime}} 2 \pi r d r=\int_{r^{\prime}=x}^{r^{\prime}=+\infty} \frac{e^{-\frac{r^{\prime}}{L}}}{2 D} d r^{\prime}
$$

Hence: $\Phi(x)=\frac{S L}{2 D} e^{-\frac{x}{L}}$

Fig. 10.21 Integration over the loops


Equation 10.17 is obtained as was shown earlier (Fig. 10.21).
This principle of superposing the solutions will be employed later for the case of media having localized absorbing materials that can be modeled as negative sources.

### 10.7.11 Absorbing Slab in an Infinite Source Medium

Let us consider a plane source at the center of an infinite medium with a uniformly distributed source in the volume $S$; the principle of flux superposition can be applied to calculate the flux in the medium as resulting from:

- a constant flux $S / \Sigma_{a}$ in the infinite medium without taking into account the plane source ( $S$ in $n / \mathrm{cm}^{3} / \mathrm{s}$ ).
- a flux $\Phi(x)=S_{P} L e^{-\frac{|x|}{L}} /(2 D)$ emitted by the plane with the uniformly distributed source $S_{P}$ in $n / \mathrm{cm}^{2} / \mathrm{s}$.

If the plane is absorbing (Fig. 10.22) instead of being a source, it can be assumed that neutrons are lost and there is thus a negative source. If the flux in the plane is equal to $\Phi_{p}$ and the thin slab has a thickness $\Delta x_{p}$, the neutron loss is equal to the absorption rate in the slab:

$$
S_{p}=\Sigma_{a} \Phi_{p} \Delta x_{p}
$$

thereby leading to the flux expression in the medium as:

$$
\Phi(x)=\frac{S}{\Sigma_{a}}-\frac{S_{P}}{2} \frac{L}{D} e^{-\frac{|x|}{L}}=\frac{S}{\Sigma_{a}}-\frac{\Phi_{p} \Delta x_{p}}{2 L} e^{-\frac{|x|}{L}}
$$

Fig. 10.22 Absorbing plane in a source medium


### 10.7.12 Thin Absorbing Slabs, the Galanin Method

In the concept of source sinks by A.D. Galanin ${ }^{7}$ (Galanin 1960), the absorption of an infinitely thin slab is modeled as a negative source. We wish to compute the effect of the flux (produced by a source at the origin) from identical absorbing slabs, each of negligible thickness, placed in a scattering and absorbing medium. To do so, the diffusion equation is written as follows, using the Dirac delta function $\delta(x)$ to model the source at the origin:

$$
-D \frac{d^{2} \Phi(x)}{d x^{2}}+\Sigma_{a} \Phi(x)+\gamma \Phi_{l} \delta\left(x-x_{l}\right)=S \delta(x)
$$

This equation introduces an intensity coefficient $\gamma$ called the Galanin coefficient ${ }^{8}$ as well as the flux of the slabs $\Phi_{l}$ at positions $x_{l}$. It can be solved by applying the Fourier transform:

$$
\bar{\Phi}(u)=\int_{-\infty}^{+\infty} \Phi(x) e^{-i 2 \pi u x} d x
$$

which is applied to the diffusion equation, given that $\bar{\delta}(u)=1$, $\overline{\delta_{x-x_{l}}}(u)=e^{-i 2 \pi u x_{l}}$ and $\frac{\overline{d^{2} \Phi}}{d x^{2}}=4 \pi^{2} u^{2} \bar{\phi}$ :

[^240]

Fig. 10.23 Lattice of absorbing slabs in a scattering/absorbing medium with a source

$$
\bar{\Phi}=\frac{1}{4 \pi^{2} D u^{2}+\Sigma_{a}}\left(S-\gamma \sum_{l} \Phi_{l} e^{-i 2 \pi u x_{l}}\right)
$$

Application of the inverse Fourier transform to the previous equation leads to:

$$
\Phi(x)=\frac{S L}{2 D} e^{-\frac{凶 x}{L}}-\frac{\gamma L}{2 D} \sum_{l} \Phi_{l} e^{-\frac{|-x-x|}{L}}
$$

The fluxes in the slabs $\Phi_{m}$ at positions $x_{m}$ are given by a system of linear equations that can be solved numerically for a finite number of slabs:

$$
\forall m \in]-\infty,+\infty\left[, \quad \Phi_{m}=\frac{S L}{2 D} e^{-\frac{\mid x}{L}}-\frac{\gamma L}{2 D} \sum_{l} \Phi_{l} e^{-\frac{\left|x_{m}-x\right| x \mid}{L}}\right.
$$

In the particular case of an infinite lattice that is regularly spaced with slabs of similar Galanin constant, Cassel and Williams ${ }^{9}$ devised an elegant analytical solution that is beyond the scope of this work (Fig. 10.23).

### 10.7.13 Flux Transient

Supposing that a time-dependent source is imposed, the transient nature implies that the flux will naturally depend on time. Indeed, the diffusion equation in plane geometry with a fission source is written as:

[^241]$$
\frac{1}{v} \frac{\partial \Phi(x, t)}{\partial t}-D \Delta \Phi(x, t)+\Sigma_{a} \Phi(x, t)=\nu \Sigma_{f} \Phi(x, t)
$$

Using the hypothesis of variable separation for space and time, the following equation is reached:

$$
\Phi(x, t)=\psi(x) \phi(t)
$$

Injecting this decomposition in the diffusion equation, then, separating the problem into a term depending on time only and another only on space, we obtain:

$$
\left\{\begin{array}{l}
\frac{1}{\varphi(t)} \frac{\partial \varphi(t)}{\partial t}=-\lambda_{k} \\
\frac{v}{\psi(x)}\left[D \Delta \psi(x)+\left(\nu \Sigma_{f}-\Sigma_{a}\right) \psi(x)\right]=-\lambda_{k}
\end{array}\right.
$$

The choice of an arbitrarily negative constant $-\lambda_{k}$ as solution to the problem will be discussed later on. The pure spatial equation for $\varphi(x)$ can be solved using an approach with eigenfunctions of the Laplace operator for the homogeneous problem as seen earlier, i.e.:

$$
D \Delta \psi(x)+\left(\frac{\lambda_{k}}{v}+\nu \Sigma_{f}-\Sigma_{a}\right) \psi(x)=0
$$

with: $\psi(x)=\sum_{k=1}^{\infty} \psi_{k} \Phi_{k}(x)$ and $\Delta \Phi_{k}(x)+B_{k}^{2} \Phi_{k}(x)=0$
For a slab of thickness $a$, the eigenfunctions that are equal to zero at the boundaries of the slab are of the following form:

$$
\Phi_{k}(x)=\varphi_{k} \cos \left(\frac{k \pi}{a} x\right)
$$

The index and the sign of $-\lambda_{k}$ are thus significant at this point since the following boundary conditions $\psi(a / 2)=0$ and $\psi(-a / 2)=0$ will be applied:

$$
\lambda_{k}=v\left(D B_{k}^{2}+\Sigma_{a}-\nu \Sigma_{f}\right) \quad k \text { odd }
$$

The general solution is of the form:

$$
\Phi(x, t)=\sum_{k=1}^{\infty} \varphi_{k} e^{-\lambda_{k} t} \Phi_{k}(x)
$$

By summing only on the odd $k$ values if the solution sought is zero at the boundaries of the slab. Using the orthogonality property of eigenfunctions and the initial value of the flux, the following can be inferred:

$$
\varphi_{k}=\frac{2}{a} \int_{-\frac{a}{2}}^{+\frac{a}{2}} \Phi(x, 0) \Phi_{k}(x) d x \quad \text { with: } \quad \Phi(x, 0)=\sum_{k=1}^{\infty} \varphi_{k} \Phi_{k}(x)
$$

Thus, we obtain:

$$
\Phi(x, t)=\sum_{k=1}^{\infty} \frac{2}{a} \int_{-\frac{a}{2}}^{+\frac{a}{2}} \Phi\left(x^{\prime}, 0\right) \Phi_{k}\left(x^{\prime}\right) d x^{\prime} e^{-\lambda_{k} t} \Phi_{k}(x)
$$

(Duderstadt and Hamilton 1976) point out that this flux is not really separable as a product of functions depending on space and time due to the infinite sum, despite the hypothesis that the fundamental modes $e^{-\lambda_{k} t} \Phi_{k}(x)$ are separable. It should also be noted that the existence of a stationary solution requires that the coefficient $\lambda_{1}$ be equal to zero, leading to a criticality condition, which will be discussed in the next chapter:

$$
B_{1}^{2}=\left(\frac{\pi}{a}\right)^{2}=\frac{\nu \Sigma_{f}-\Sigma_{a}}{D}
$$

Increasing the eigenvalues $B_{k}^{2}$ for increasing $k$ values leads to an increase of $\lambda_{k}$, thereby reducing gradually the contribution of the terms $e^{-\lambda_{k} t}$. If the reactor is over-critical, i.e. material buckling $\left(\nu \Sigma_{f}-\Sigma_{a}\right) / D$ is greater than geometrical buckling (the first and smallest positive eigenvalue):

$$
\frac{\nu \Sigma_{f}-\Sigma_{a}}{D}>B_{1}^{2}=\left(\frac{\pi}{a}\right)^{2}
$$

The existence of a positive $\lambda_{1}$ is thus assured, leading to an increase in flux that will adopt the shape of the fundamental mode with the decay of the other modes. This phenomenon will be discussed later in the chapter on reactor kinetics. It should be noted that if:

$$
\frac{\nu \Sigma_{f}-\Sigma_{a}}{D}>B_{3}^{2}=\left(\frac{3 \pi}{a}\right)^{2}
$$

a second harmonic with coefficient $\lambda_{3}$ will appear. For a sub-critical reactor, all constants $\lambda_{k}$ are negative and the flux, for any initial value, will tend towards 0 .

### 10.8 Measurement of the Scattering Path of a Moderator by Attenuation

(Meghreblian and Holmes 1960, p226)
The equations studied earlier allow calculation of the value of $L$ for simple geometries, such as the plane source in infinite medium, by measuring the exponential attenuation of thermal neutrons. In reality, this theoretical situation with an infinite hypothesis is never encountered. The usual technique set up in this case, devised by Enrico Fermi (Stephenson 1954, p141; Barjon 1993, p18; Glasstone and Edlund 1972, p117 and p281; Stacey 2001, p56; Glasstone and Sesonske 1994, p147; Bekurts and Wirtz 1964, p360) consists in carrying out an experiment in which thermal neutrons are injected at the base of a prism with a square or rectangular cross section, and of a height much greater than the length of the side (Fig. 10.24).

The diffusion equation may then be solved for this geometry:

$$
\Delta \Phi(x, y, z)-\frac{1}{L^{2}} \Phi(x, y, z)=0
$$

such that the three space variables can be separated:

$$
\Phi(x, y, z)=\varphi(x) \varphi(x) \psi(z)
$$

The diffusion equation can then be written in the following form:

$$
\frac{\frac{d^{2} \phi}{d x^{2}}}{\phi(x)}+\frac{\frac{d^{2} \phi}{d y^{2}}}{\phi(y)}+\frac{\frac{d^{2} \psi}{d z^{2}}}{\psi(z)}-\frac{1}{L^{2}}=0
$$

which has a solution only if:

$$
\frac{d^{2} \phi}{d x^{2}}+B_{x}^{2} \phi(x)=0, \quad \frac{d^{2} \phi}{d y^{2}}+B_{y}^{2} \phi(y)=0 \quad \text { and } \quad \frac{d^{2} \psi}{d z^{2}}+B_{z}^{2} \psi(z)=0
$$

with: $B_{x}^{2}+B_{y}^{2}+B_{z}^{2}=\frac{1}{L^{2}}$
The solution is sought for the fundamental mode that is equal to zero at the surface of the prism in directions $x$ and $y$, and retaining only the decreasing exponential along the $z$ axis (by considering that the height $c$ is a very large compared to the width $a$ and the length $b$ ). Thus, the solution that is zero at infinity is written in the form:

$$
\Phi(x, y, z) \approx \sum_{k} \sum_{m} \Phi_{k m} \cos \left(k \pi \frac{x}{a}\right) \quad \cos \left(m \pi \frac{y}{b}\right) e^{-\frac{z}{L_{k m}}}
$$

For a column of finite extrapolated height $z_{0}$, the solution may be written as:


Fig. 10.24 Moderator prism for the measurement of $L$

$$
\Phi(x, y, z)=\sum_{k} \sum_{m} \Phi_{k m} \cos \left(k \pi \frac{x}{a}\right) \quad \cos \left(m \pi \frac{y}{b}\right) \operatorname{sh}\left[\kappa_{k m}\left(z_{0}-z\right)\right]
$$

Due to the symmetries, it can be anticipated that coefficients $\Phi_{k m}$ are zero where $k$ or $m$ are even. The source can be modeled as a plane source $S \delta(x, y) / 2$ where the Dirac delta for two dimensions is expanded in a Fourier series:

$$
\begin{gathered}
\delta(x, y)=\sum_{k} \sum_{m} \frac{4}{a b} \cos \left(k \pi \frac{x}{a}\right) \cos \left(m \pi \frac{y}{b}\right) \\
\text { with: } \quad \int_{-\frac{a}{2}}^{+\frac{a}{2}} \int_{-\frac{b}{2}}^{+\frac{b}{2}} \delta(x, y) d x d y=1
\end{gathered}
$$

The coefficient 2 is applied to the source since only $S / 2$ neutrons are emitted towards the prism. The coefficients $\Phi_{k m}$ are found by identification of the coefficients of the axial diffusion current to the source:

$$
\begin{aligned}
-D\left(\frac{\partial \Phi}{\partial z}\right)_{0} & =D \sum_{k} \sum_{m} \frac{\Phi_{k m}}{L_{k m}} \cos \left(k \pi \frac{x}{a}\right) \cos \left(m \pi \frac{y}{b}\right) \\
& =\frac{S}{2} \sum_{k} \sum_{m} \frac{4}{a b} \cos \left(k \pi \frac{x}{a}\right) \cos \left(m \pi \frac{y}{b}\right)
\end{aligned}
$$

$$
\text { where: } \quad \Phi_{k m}=\frac{2 S L_{k m}}{D a b}
$$

The fundamental mode is obtained for $k=1$ and $m=1$, with the other harmonics being damped very quickly as we move further from the source. If the flux is measured far from the source, $L$ can be computed as:

$$
\frac{1}{L^{2}}=\frac{1}{L_{11}^{2}}-\left(\frac{\pi}{a}\right)^{2}-\left(\frac{\pi}{b}\right)^{2}
$$

The terms $(\pi / a)^{2}$ and $(\pi / b)^{2}$ are bucklings that characterize the radial leakage from the prism. The harmonics disappear very quickly far from the source. An experiment to measure the scattering path in graphite of nuclear quality using this method was set up in 1966 with the French MARIUS graphite pile. ${ }^{10}$

A square-based column was placed at the side of the MARIUS pile and the column was protected from parasite neutrons emanating from the pile-from the external parts at the beginning of the column (Faraday cage effect using an electrical analogy, cf. (Figs. 10.25 and 10.26) -using cadmium logs. Analysis showed the absence of a harmonic of order 3 at a distance of 50 cm from the source. The scattering length of the graphite was $L=51.98 \pm 0.36 \mathrm{~cm}$ as measured experimentally for reference conditions ( $T=20^{\circ} \mathrm{C}, \rho=1.672 \mathrm{~g} / \mathrm{cm}^{3}$ and pressure $=738.8 \mathrm{~mm} \mathrm{Hg}$ ) and the absorption cross section of the graphite was $\sigma_{a}=3.92 \pm 0.06$ mbarns. A similar analysis can be carried out with a cylinder, expressing the flux as:

$$
\Phi(r, \theta, z)=\sum_{k} \sum_{m} \Phi_{k m} J_{k}\left(J_{k m} \frac{r}{R}\right) \quad \cos (m \theta) \operatorname{sh}\left[\kappa_{k m}\left(z_{0}-z\right)\right]
$$

The pulsed source method conceived by J. Horowitz and V. Raievski (Raievski 1960) is an original method to compute the scattering length. It consists in oscillating a source in periodic fashion using a mechanical means. The resulting source has the form $e^{i \omega t} S(\vec{r})$. The solution to the non-stationary diffusion equation in the column:

$$
-D \Delta \Phi(\vec{r}, t)+\Sigma_{a} \Phi(\vec{r}, t)=-\frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t}
$$

has a flux solution of the form $\Phi(\overrightarrow{r, t})=e^{i \omega t} \varphi(\vec{r})$. By inserting this form in the differential equation and assuming that there is a point source, the general solution can be established as:

$$
\varphi(\vec{r})=\alpha \frac{e^{+i \mu r}}{r}+\beta \frac{e^{-i \mu r}}{r}
$$

with: $\mu^{2}=\frac{1}{L^{2}}+i \frac{\omega}{D v}$

[^242]

Fig. 10.25 Longitudinal cross section and front view of the square-based graphite column placed at the side of the Marius pile (Cadarache (France), 1966). The position of the protective cadmium logs can be observed


Fig. 10.26 Sketch of the French MARIUS reactor. The moving train used for oscillation experiments is seen
which is usually written as: $\mu=\sqrt{\frac{\frac{1}{L^{2}}+m^{2}}{2}+i \sqrt{-\frac{\frac{1}{L^{2}}+m^{2}}{2}}}$
with $m^{2}=\sqrt{\frac{1}{L^{4}}+\left(\frac{\omega}{D v}\right)^{2}}$
The flux then behaves like a spherical wave of the following type:

$$
\left.\Phi(\vec{r}, t) \propto \frac{e^{ \pm i \eta r}}{r} e^{i\left(\omega t-\frac{2 \pi}{\lambda} r\right.}\right)
$$

with attenuation coefficient $\eta$, wavelength $\lambda$ and propagation speed $v$ :

$$
\eta=\sqrt{\frac{\frac{1}{L^{2}}+m^{2}}{2}} \quad \lambda=2 \pi \sqrt{\frac{2}{m^{2}-\frac{1}{L^{2}}}} \quad v=\omega \sqrt{\frac{2}{m^{2}-\frac{1}{L^{2}}}}
$$

Measurement of these quantities is performed with detectors placed along the axis of the column. This allows evaluation of the scattering length and the diffusion coefficient. That method was applied to the same graphite column placed at the side of the MARIUS reactor, and yielded a scattering length $L=51.70 \pm 0.25 \mathrm{~cm}$, $v \Sigma_{a}=77.2 \pm 0.6 \mathrm{~s}^{-1}$, a mean free path with transport correction of $\lambda_{t r}=2.497$ $\pm 0.01 \mathrm{~cm}$, and an absorption cross section for graphite of $\sigma_{a}=3.97 \pm 0.03$ mbarns, which is consistent with the previous exponential experiment.

### 10.9 Pulsed Neutron Method

The concept of using a pulsed neutron source in a scattering medium is very old. The golden days of the physics of pulsed neutron date back to 1955-1965. Indeed, study of neutron thermalization in a scattering medium may be readily performed by an experimenter having a neutron source and an adequate counting/acquisition system. The French CEA thus carried out several measurements of graphite to obtain its properties, in support of the French UNGG program. Furthermore, similar measurements were carried out on water for comparison with foreign laboratories and for the design of methods. In this context, the work of V. Raievski and J. Horowitz for measuring the asymptotic diffusion coefficient of heavy water published on the occasion of the Atoms for Peace conference at Geneva in 1955 may be cited.

The pulsed neutron method was first employed by Manley et al. ${ }^{11}$, who used it to measure prompt neutron lifetime in water and the cross section of hydrogen. The results were published in 1942 in Physical Review and before the interruption in publications on nuclear energy due to the Manhattan project. The pulsed neutron

[^243]method was extensively developed in the United States after the war. ${ }^{12}$ France followed in the 1960s.

In 1955, J. Lehner and G.M. Wing ${ }^{13,14}$ proposed a complete theoretical approach for the spectrum (in the mathematical sense) of functions that are solutions to the neutron transport equation for neutrons, with an asymptotic slowing-down operator in the case of an infinite slab. G. Milton Wing took over and developed an analytical solution for the kinetic transport problem in Chap. 8 of his book of 1962: An introduction to transport theory (Wing 1962). S. Albertoni and B. Montagnini ${ }^{15}$ reviewed the main results and extended them to other forms of operators in an excellent paper published in 1965 during the IAEA symposium at Karlsruhe on the physics of pulsed neutrons. Lehner and Wing showed that the neutron flux solution of the slowing-down equation in kinetics can be decomposed using a spectrum of functions (in distribution terms), and consisting of:

- a continuous spectrum in the complex half-space of eigenvalues for which the real part is less than $-\Sigma_{t} v_{0}$, where $v_{0}$ is the speed of the neutron and $\Sigma_{t}$ is the total cross section of the slab,
- a finite number of strictly positive eigenvalues.

Wing showed in his book that neutron density can be written as (Wing 1962, p125):

$$
n(z, \mu, t)=\sum_{i=1}^{m} e^{\left(\beta_{i}-1\right) t} \sum_{k=1}^{s_{j}}\left(f, \Psi_{i, k}^{*}\right) \Psi_{i, k}(z, \mu)+e^{-t} \zeta(z, \mu, t)
$$

The function $\zeta(z, \mu, t)$ accounts for the continuous spectrum while the discrete spectrum of eigenvalues $\lambda_{i}=\beta_{i}-1$ appears under the summation sign. The function $\zeta(z, \mu, t)$ is bounded by:

$$
|\zeta(z, \mu, t)|<D_{1}(z, \mu) t^{2} \ln ^{2} t
$$

The calculation of this bound is extremely important since it leads to the affirmation that:

$$
\lim _{t \rightarrow+\infty} e^{-t} \zeta(z, \mu, t)=0
$$

The decay of the function $\zeta(z, \mu, t)$ over time is a very complex problem, but it is reasonable to suppose that it is rapidly negligible compared to the largest discrete eigenvalue. Thus, in the end, we may consider that neutron density behaves as

[^244]$e^{\max \left(\lambda_{i}\right) t}$, whilst noticing that all values of $\lambda_{i}$ are negative. For a finite medium, Lehner and Wing showed that the continuous spectrum degenerates into a spectrum with complex discrete eigenvalues, while conserving strictly real eigenvalues above $-\Sigma_{t} v_{0}$. This remark removes the problem of the continuous spectrum in an asymptotic approach over long periods.

It is also very interesting to compare this theory with treatment of the 1D transport equation as a function of the cosine of the scattering angle $\mu$ in the theory of Lafore and Millot or of Case for the solution of the dispersion equation.

In a finite medium, in which flux may be factorized as an infinite sum of decreasing exponentials, flux behaves "very quickly" as a unique decreasing exponential. This property is used to write:

$$
\Phi(\vec{r}, E, t) \propto \Phi(\vec{r}) \quad \Phi_{\lambda}(E) e^{-\lambda t}
$$

The letter $\Phi$ is always used regardless of its dependence (space, energy or time) so as to simplify the notations (thereby avoiding the use of too many letters!).

The time-dependent equation under its diffusion form is:

$$
\begin{aligned}
& \frac{1}{v} \frac{\partial \Phi(\vec{r}, E, t)}{\partial t}-D(\vec{r}, E) \Delta \Phi(\vec{r}, E, t)+\Sigma_{t}(\vec{r}, E) \Phi(\vec{r}, E, t)= \\
& \quad \int_{E^{\prime}} d E^{\prime} \Sigma_{s}\left(\vec{r}, E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}, t\right)+S(\vec{r}, E, t)
\end{aligned}
$$

In a non-multiplying medium, the source is zero. The RHS of the equation is the slowing-down operator:

$$
R[\Phi] \equiv \int_{E^{\prime}} d E^{\prime} \Sigma_{s}\left(\vec{r}, E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}, t\right)
$$

The equation for diffusion without source can be overwritten by distinguishing the scattering reactions from absorption in the total cross section:

$$
\begin{aligned}
\frac{1}{v} \frac{\partial \Phi(\vec{r}, E, t)}{\partial t}-D(\vec{r}, E) \Delta \Phi(\vec{r}, E, t)+\Sigma_{a}(\vec{r}, E) & \Phi(\vec{r}, E, t)= \\
& R[\Phi]-\Sigma_{s}(\vec{r}, E) \Phi(\vec{r}, E, t) \equiv H[\Phi]
\end{aligned}
$$

Assuming that the spatial part of the flux obeys the fundamental mode, i.e.:

$$
\Delta \Phi(\vec{r})+B^{2} \Phi(\vec{r})=0
$$

By injecting this form of the flux in the diffusion equation, the following is obtained:

$$
\left(-\frac{\lambda}{v}+D B^{2}+\Sigma_{a}\right) \Phi_{\lambda}(E)=H\left[\Phi_{\lambda}(E)\right]
$$

This equation is for the eigenfunction in energy. By integrating it for all energies, the following property of the $H$ operator may be employed:

$$
\int_{E} H\left[\Phi_{\lambda}(E)\right] d E=0
$$

Since by definition:

$$
\int_{E} d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right)=\Sigma_{s}\left(E^{\prime}\right)
$$

By considering that absorption has a pure $1 / v$ form, we obtain:

$$
-\lambda+\overline{D v} B^{2}+v_{T} \Sigma_{a}(k T)=0
$$

since $\overline{D v} \equiv \frac{\int_{v} n(v) D v d v}{\int_{v} n(v) d v}$
For an infinite medium $\left(B^{2}=0\right)$, the solution is a pure Maxwellian flux given that:
$-\lambda+v_{T} \Sigma_{a}(k T)=0$ and thus $H\left[\Phi_{\lambda}(E)\right]=0$
For cases where $B^{2}>0$, the flux is shifted towards lower energies: this is called cooling of the neutron spectrum. In the opposite case where $B^{2}<0$, the flux is shifted towards the higher energies; this is called hardening or warming of the spectrum. $\overline{D v}\left(B^{2}\right)$ can be expressed as a continuous function of buckling in its polynomial form:

$$
\overline{D v}\left(B^{2}\right)=D_{0}-C B^{2}-F B^{4}+\ldots
$$

Thus, the following expanded expression for the eigenvalue:

$$
\lambda\left(B^{2}\right)=v_{0} \Sigma_{a}(k T)+D_{0} B^{2}-C B^{4}+F B^{6}+\ldots
$$

Several authors have thus employed this formulation to experimentally measure:

- the neutron lifetime in the moderator being considered $\left(1 / v_{0} \Sigma_{a}(k T)\right)$,
- the asymptotic diffusion coefficient ${ }^{16} D_{0\left[\mathrm{~cm}^{2} / \mathrm{s}\right]}$, not to be confused with the usual diffusion coefficient, which is expressed in cm ,
- the cooling coefficient $C_{\left[\mathrm{cm}^{4} / \mathrm{s}\right]}$,
- or the coefficient $F_{\left[\mathrm{cm}^{6} / \mathrm{s}\right]}$ which is negative for water.

[^245]In his review of pulsed neutrons experiments, ${ }^{17}$ K.H. Beckurts presents the two main methods of measuring $\lambda\left(B^{2}\right)$. For $B^{2}>0$, the size of the moderator being studied is varied to change the buckling. It should be noted that it is difficult to conduct experimental measurement of very extensive buckling, which occurs in small reactors. The buckling for $B^{2}<0$ can be measured by gradually poisoning the moderator with an absorbing material; this can be quite easily achieved for example by adding boric acid to the water. The spatial attenuation coefficient $\kappa$, such that $\Phi(\vec{r}, E)=e^{-\kappa z} \Phi_{\kappa}(E)$, then depends on the absorption of the medium (Figs. 10.27 and 10.28):

$$
\kappa^{2}=A_{1} \Sigma_{a}(k T)+A_{2} \Sigma_{a}^{2}(k T)+\ldots
$$



Schematic of the functions $\alpha\left(B^{2}\right)$ and $\kappa^{2}\left[v_{0} \Sigma_{a}(k T)\right]$.
Fig. 10.27 Schematic of the functions $\alpha$ and $\kappa^{2}$. Adapted from Henry C. Honeck: Brookhaven Conference, volume IV, p1208 (1962)

[^246]

The enlarged $\alpha$ versus $B^{2}$ curve for $\mathrm{H}_{2} \mathrm{O}$
Fig. 10.28 The enlarged alpha versus B square curve for water. Adapted from K.H. Beckurts, Karlsruhe Conference, Vol. 1, p 10 (Beckurts 1965)

These experimental measurements can be compared to theoretical calculations using an explicit representation for the slowing-down operator (e.g. the Nelkin model)-this was a vast area of research in the 1960s.

In France, at the beginning of the 60 's, for his PhD Gérard Cuny ${ }^{18}$ performed experiments to determine $1 / v_{0} \Sigma_{a}(k T)_{[\mu s]}$ and $D_{0}\left(T_{H_{2} O}\right)_{\left[c m^{2} / s\right]}$ by modifying the buckling of a vessel of water, for which the height was varied. The parameter $C$ could not be measured due to the unsophisticated counting system of the time, $C$ being calculable only if $1 / v_{0} \Sigma_{a}(k T)_{[\mu s]}$ and $D_{0}\left(T_{H_{2} O}\right)_{\left[\mathrm{cm}^{2} / s\right]}$ are known with sufficient precision. The value of his work lies in analysis of the error on the eigenvalue due to the count rate and on the precision concerning time for the permanent regime to be established. This measuring technique was later used by the CEA at Cadarache ${ }^{19}$ for graphite with V. Deniz and M. Sagot. The measurements for $D_{0}\left(T_{H_{2} O}\right)_{\left[\mathrm{cm}^{2} / \mathrm{s}\right]}$ are consistent with the existing literature at that time, especially those of Dardel and N.G. Sjöstrand, who set the standards for such experiments.

Two conferences are indispensable for the historical review of pulsed neutrons. The first one on the thermalization of neutrons took place at Brookhaven (April 30 to May 2, 1962) and involved the greatest names in the field: Corngold, Sjöstrand, Starr, Beckurts, etc. Volumes III and IV dealing with the theoretical aspects are extremely useful. The second was the major meeting organized by the IAEA at Karlsruhe (May 10-14, 1965), which gives a more recent overview of the field.

### 10.10 Diffusion in a Homogeneous Slab

Let us consider the calculation of the flux at two energy groups in an infinite slab due to an incident flux of monokinetic neutrons (source $S$ at energy $E_{0}=10 \mathrm{MeV}$ for instance) perpendicular to the slab. The energy spectrum is discretized into two groups: fast at [ $10 \mathrm{MeV}, 0.625 \mathrm{eV}$ [ and thermal at [ $0.625 \mathrm{eV}, 0 \mathrm{eV}$ [ by assuming that there is no upscattering from the thermal group to the fast group. Thus, the diffusion equation is written for two energy groups as (Fig. 10.29):

$$
\left\{\begin{array}{l}
-D_{1} \Delta \Phi_{1}+\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) \Phi_{1}=S \delta(x) \\
-D_{2} \Delta \Phi_{2}+\Sigma_{a 2} \Phi_{2}=\Sigma_{1 \rightarrow 2} \Phi_{1}
\end{array}\right.
$$

[^247]

Fig. 10.29 Scattering in a slab of water in two-group theory : fast and thermal flux along the depth in the slab
a differential system that is solved by seeking the flux solutions that cancel one another out at infinity. If we set $\kappa_{1}^{2}=\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) / D_{1}, \kappa_{2}^{2}=\Sigma_{a 2} / D_{1}$ and $\Sigma_{t 1}=\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}$, by considering that the source is a neutron current in the positive direction (abscissa) $\left(J_{1}^{+}(0)=S\right)$ and supposing that the thermal flux is zero at the origin, we obtain:

$$
\left\{\begin{array}{l}
\Phi_{1}(x)=\frac{S}{\kappa_{1} D_{1}} e^{-\kappa_{1} x} \\
\Phi_{2}(x)=\frac{\Sigma_{1 \rightarrow 2} S}{\kappa_{1} D_{1} D_{2}\left(\kappa_{1}^{2}-\kappa_{2}^{2}\right)}\left(e^{-\kappa_{2} x}-e^{-\kappa_{1} x}\right)
\end{array}\right.
$$

These results lead to several remarks: the fast flux decays exponentially and conserves the current at the origin as imposed by the boundary condition. The fast flux at the origin is equal to $S /\left(\kappa_{1} D_{1}\right)=S / \sqrt{\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) D_{1}}$. For pure water at $20^{\circ} \mathrm{C}$, (Barjon 1993) gives $D_{1} \approx 1.16 \mathrm{~cm}, \Sigma_{1 \rightarrow 2} \approx 0.043 \mathrm{~cm}^{-1}$ and $\Sigma_{a 1} \ll \Sigma_{1 \rightarrow 2}$, which means that the fast flux at the origin is larger than the flux $S$.

This result may be taken to show that fast neutrons with energy of less than $E_{0}$ are back-scattered by the water slab and leak in the vacuum. These neutrons traveling through the surface of the slab towards the left must be counted with neutrons at $E_{0}=10 \mathrm{MeV}$ traveling towards the right. The rise in the thermal flux is physical and predicts the leakage of thermal neutrons towards the vacuum. This is the albedo effect that will be discussed in more detail in the chapter on the reflector.

The solution obtained can be improved by noticing that 10 MeV neutrons will always move from left to right since in the case of a collision that changes their direction, eventually towards the rear, they would lose their energy. This reasoning implies that there is no 10 MeV neutron able to escape towards the vacuum, meaning that the current $J_{0}^{-}(x=0)=J_{0}^{-}(x)=0$, where 0 indicates energy $E_{0}$. Hence, the positive flux and currents can be calculated precisely in the water slab. The latter flux and current are attenuated exponentially due to absorption and scattering:

$$
\left\{\begin{array}{l}
\Phi_{0}(x)=\Phi_{0}(0) e^{-\Sigma_{10} x}=S e^{-\Sigma_{10} x} \\
J_{0}^{+}(x)=J_{0}^{+}(0) e^{-\Sigma_{00} x}=S e^{-\Sigma_{10} x}
\end{array}\right.
$$

It may be noted that neutrons at this energy are mono-directional, and that flux and current are the same. This result is trivial in transport theory and is compatible with the diffusion equation only if:

$$
J(x)=J_{0}^{+}(x)-\underbrace{J_{0}^{-}(x)}_{0}=S e^{-\Sigma_{t 0} x}=-D_{0} \operatorname{grad} \Phi_{0}=D_{0} \Sigma_{t 0} S e^{-\Sigma_{t 0} x}
$$

for which equality is possible only by imposing as the diffusion coefficient $D_{0}=$ $1 / \Sigma_{t 0}$, i.e. the mean free path. This result, which is diverges greatly from the traditional theory ( $D=1 /\left(3 \Sigma_{t}\right)$ ), proves that diffusion is only applicable by construction if the flux results from a diffusing process. This is not the case for a beam of neutrons. In any case, it is not correct to write the diffusion equation for the flux $\Phi_{0}$, however far the source be. Assuming this artificial diffusion coefficient $D_{0}$, the flux at 10 MeV obeys a classical transport equation with $\kappa_{0}^{2}=\left(\Sigma_{a 0}+\Sigma_{0 \rightarrow 1}\right) / D_{0}$ :

$$
-D_{0} \Delta \Phi_{0}+\underbrace{\left(\Sigma_{a 0}+\Sigma_{0 \rightarrow 1}\right)}_{\Sigma_{10}} \Phi_{0}=S \delta(x) \text { with } \Phi_{0}(x)=\frac{S}{\kappa_{0} D_{0}} e^{-\kappa_{0} x}=S e^{-\Sigma_{10} x} \text { as a }
$$

solution
Since a particular energy $E_{0}$ for the fast group has been defined, the fast group is defined as ] $10 \mathrm{MeV}, 0.625 \mathrm{eV}[$ where the first bound is excluded. The equation in this new group must contain a source term for scattering reaction rates of energy $E_{0}$ to group 1:

$$
-D_{1} \Delta \Phi_{1}+\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) \Phi_{1}=\Sigma_{0 \rightarrow 1} \Phi_{0}=\Sigma_{0 \rightarrow 1} S e^{-\Sigma_{t 0} x}
$$

for which the solution is zero at 0 and which is written as $\kappa_{1}^{2}=\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) / D_{1}$ :

$$
\Phi_{1}(x)=\frac{\Sigma_{0 \rightarrow 1} S}{D_{1}\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)}\left(e^{-\Sigma_{t 0} x}-e^{-\kappa_{1} x}\right)
$$

Assuming that there is no scattering directly from energy $E_{0}$ to group 2 (this is not completely physically correct for slowing-down with hydrogen from water but remains very acceptable in terms of order of magnitude ${ }^{20}$ ), the diffusion equation in the thermal group is unchanged. Its solution is given by:

[^248]

Fig. 10.30 Scattering in a slab of water in two-group diffusion theory + transport source

$$
\Phi_{2}(x)=\frac{\Sigma_{0 \rightarrow 1} \Sigma_{1 \rightarrow 2} S}{D_{1} D_{2}\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)}\left(\frac{e^{-\kappa_{2} x}-e^{-\kappa_{1} x}}{\left(\kappa_{2}^{2}-\kappa_{1}^{2}\right)}-\frac{e^{-\kappa_{2} x}-e^{-\Sigma_{t 0} x}}{\left(\kappa_{2}^{2}-\Sigma_{t 0}^{2}\right)}\right)
$$

These results remain a two-energy group calculation but integrate a source at energy $E_{0}$ as evaluated by transport (Fig. 10.30). It is known from theory that the flux $\Phi_{1}$ and $\Phi_{2}$ are false as we tend towards the source at least three times the mean free path of the neutron. Hence, we cannot place too much trust in the value for the completed total flux as given by $\Phi_{\text {total }}=\Phi_{0}^{\text {transport }}+\Phi_{1}^{\text {diffusion }}+\Phi_{2}^{\text {diffusion }}$ close to the source.

Diffusion theory predicts that the neutron current in the negative direction (leakage from the slab) can be computed with a neutron balance on the slab for both the fast and thermal groups. This balance is synonymous with the fact that the number of fast neutrons leaking from the slab is the difference between the fast source and the number of fast neutrons absorbed or scattered in the thermal group:

$$
\begin{aligned}
\int_{0}^{+\infty}-D_{1} \Delta \Phi_{1}(x) d x & =\int_{0}^{+\infty} \Sigma_{0 \rightarrow 1} S e^{-\Sigma_{t 0} x} d x-\int_{0}^{+\infty}\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) \Phi_{1}(x) d x \\
& =\frac{\Sigma_{0 \rightarrow 1}}{\Sigma_{t 0}} S\left[1-\frac{\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right)}{\kappa_{1} D_{1}\left(\kappa_{1}+\Sigma_{t 0}\right)}\right]=\frac{\Sigma_{0 \rightarrow 1}}{\left(\kappa_{1}+\Sigma_{t 0}\right)} S
\end{aligned}
$$

This leakage can also be calculated by evaluating the net fast current at the interface for which the outward normal is $-\vec{x}$. It can be noticed that the positive fast current $J_{1}^{+}(0)$ is zero as vacuum does not send back any neutrons in the active region:

$$
J_{1}^{-}(0)=-J_{1}^{\text {net }}(0)=-\left.D_{1} \overrightarrow{g r a d} \Phi_{1}(x) \cdot(-\vec{x})\right|_{0}=\frac{\Sigma_{0 \rightarrow 1}}{\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)} S\left(\kappa_{1}-\Sigma_{t 0}\right)=\frac{\Sigma_{0 \rightarrow 1}}{\left(\kappa_{1}+\Sigma_{t 0}\right)} S
$$

These two calculations are indeed similar thanks to the Ostrogradski theorem that simplifies the calculation of the Laplacian term. Similarly, the thermal leakage can be also computed:

$$
J_{2}^{-}(0)=-J_{2}^{n e t}(0)=-\left.D_{2} \overrightarrow{g r a d} \Phi_{2}(x) \cdot(-\vec{x})\right|_{0}=\frac{\Sigma_{0 \rightarrow 1} \Sigma_{1 \rightarrow 2}}{D_{1}\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)}\left(\frac{1}{\kappa_{2}+\Sigma_{t 0}}-\frac{1}{\kappa_{2}+\kappa_{1}}\right) S
$$

The total albedo of the slab of water can be computed as follows, with $J_{0}^{+}(0)=S$ :

$$
\beta_{m u r}=\frac{J_{1}^{-}(0)+J_{2}^{-}(0)}{J_{0}^{+}(0)}=\frac{\Sigma_{0 \rightarrow 1}}{\left(\kappa_{1}+\Sigma_{t 0}\right)}+\frac{\Sigma_{0 \rightarrow 1} \Sigma_{1 \rightarrow 2}}{D_{1}\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)}\left(\frac{1}{\kappa_{2}+\Sigma_{t 0}}-\frac{1}{\kappa_{2}+\kappa_{1}}\right)
$$

Imposing zero-flux conditions for $\Phi_{1}$ and $\Phi_{2}$ at the interface is in fact quite artificial. The choice could have been to cancel these fluxes at the extrapolated surfaces for the fast and thermal groups, which will not have the same values. Since the current is not zero at the interface, the flux in transport theory cannot be zero either, which implies that there cannot be a zero flux at the interface between a fissile zone and a vacuum. Since $J_{1}^{+}(0)=0$ and $J_{2}^{+}(0)=0$, a more "physical" solution (with all the limitations that diffusion theory implies) could be one that ensures that $J_{1}^{-}(0)=\Phi_{1}(0)$ and $J_{2}^{-}(0)=\Phi_{2}(0)$. After calculations, we obtain:

$$
\left\{\begin{aligned}
\Phi_{1}(x) & =\frac{\Sigma_{0 \rightarrow 1} S}{D_{1}\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)}\left(e^{-\Sigma_{t 0} x}-\frac{1+\Sigma_{t 0} D_{1}}{1+\Sigma_{t 0} \kappa_{1}} e^{-\kappa_{1} x}\right) \\
\Phi_{2}(x) & =\frac{\Sigma_{0 \rightarrow 1} \Sigma_{1 \rightarrow 2} S}{D_{1} D_{2}\left(\kappa_{1}^{2}-\Sigma_{t 0}^{2}\right)}\left(\frac{1}{\left(\kappa_{2}^{2}-\Sigma_{t 0}^{2}\right)}\left(e^{-\Sigma_{t 0} x}-\frac{1+\kappa_{1} D_{2}}{1+\kappa_{2} D_{2}} e^{-\kappa_{2} x}\right)\right. \\
& \left.+\frac{1}{\left(\kappa_{1}^{2}-\kappa_{2}^{2}\right)} \frac{1+\Sigma_{t 0} D_{1}}{1+\kappa_{1} D_{1}}\left(e^{-\kappa_{1} x}-\frac{1+\Sigma_{t 0} D_{2}}{1+\kappa_{2} D_{2}} e^{-\kappa_{2} x}\right)\right)
\end{aligned}\right.
$$

This result must be interpreted with caution. We chose the fast and thermal flux such that at the interface, the diffusion current is equal to the flux. In fact, transport theory does not relate the current to the flux gradient. Using such an approach, the neutron leakage is modified and hence the albedo of the slab of water (Fig. 10.31).

These various calculations demonstrate the limits of diffusion theory and the difficulty of calculating a reflector such that its behavior in diffusion theory remains the same as a real reflector by conserving the results obtained via transport theory. This issue of transport-diffusion equivalence will be discussed later.


Fig. 10.31 Scattering in a slab in two-group diffusion theory in a slab of water + transport source + transport boundary conditions

### 10.11 Source Thermalization Transient in Diffusion Theory

### 10.11.1 Infinite Medium

Let us consider the time-dependent solution for a flux that is imposed by a source in a non-multiplying infinite medium. This flux verifies the equation in an infinite medium with our usual notations:

$$
\begin{aligned}
\frac{1}{v} \frac{\partial \Phi(\vec{r}, E, t)}{\partial t}= & -\left(\Sigma_{s}(E)+\Sigma_{a}(E)\right) \Phi(\vec{r}, E, t) \\
& +\int_{0}^{\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(\vec{r}, E^{\prime}, t\right) d E^{\prime}+S(\vec{r}, E, t)
\end{aligned}
$$

A small trick consists in writing the slowing-down operator in a symmetric form by dividing the flux and the source by a Maxwell function in energy. It may be recalled that the Maxwell function is the solution to the thermalization equation without absorption:

$$
\varphi(\vec{r}, E, t) \equiv \frac{\Phi(\vec{r}, E, t)}{\sqrt{m(E)}} \quad \text { and } \quad s(\vec{r}, E, t) \equiv \frac{S(\vec{r}, E, t)}{\sqrt{m(E)}}
$$

These new quantities are called the symmetrized flux and symmetrized source. This leads to the diffusion equation in infinite medium in the following form:

$$
\begin{aligned}
\frac{\partial \varphi(\vec{r}, E, t)}{\partial t}= & -v\left(\Sigma_{s}(E)+\Sigma_{a}(E)\right) \varphi(\vec{r}, E, t)+v \sqrt{m(E)} \\
& \times \int_{0}^{\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \frac{\varphi\left(\vec{r}, E^{\prime}, t\right)}{\sqrt{m\left(E^{\prime}\right)}} d E^{\prime}+s(\vec{r}, E, t)
\end{aligned}
$$

The symmetrized slowing-down operator may now be introduced as:

$$
R_{E}[\varphi] \equiv v \sqrt{m(E)} \int_{0}^{\infty} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \frac{\varphi\left(\vec{r}, E^{\prime}, t\right)}{\sqrt{m\left(E^{\prime}\right)}} d E^{\prime} \equiv \int_{0}^{\infty} K\left(E^{\prime} \rightarrow E\right) \varphi\left(\vec{r}, E^{\prime}, t\right) d E^{\prime}
$$

And by extension, the Boltzmann operator will be symmetric and real, and thus self-adjoint:

$$
H_{E}[\varphi] \equiv \int_{0}^{\infty}\left\{K\left(E^{\prime} \rightarrow E\right)-v\left(\Sigma_{s}(E)+\Sigma_{a}(E)\right) \delta\left(E-E^{\prime}\right)\right\} \varphi\left(\vec{r}, E^{\prime}, t\right) d E^{\prime}
$$

Introducing the Dirac function entails that the loss terms are included in the integral on energy. The solutions to the homogeneous equation (without any source term) and without leakage will be sought as an expansion in space over the eigenfunctions of the Boltzmann operator.

### 10.11.2 Finite Medium

By modelling the leakage term under the form: $D(E) \Delta \varphi(\vec{r}, E, t)$, the diffusion equation in a finite medium is written as:

$$
\frac{\partial \varphi(\vec{r}, E, t)}{\partial t}=\left\{H_{E}+v D(E) \Delta\right\}[\varphi]+s(\vec{r}, E, t)
$$

It should be noted that the operator $\left\{H_{E}+v D(E) \Delta\right\}[]$ is always symmetric and real, and hence is self-adjoint. For a case with leakage, the symmetrized flux and the source may be developed along the spatial modes of the diffusion equation in the geometry of material buckling $B^{2}$ being considered:
$\Delta \Phi_{n}(\vec{r})+B^{2} \Phi_{n}(\vec{r})=0 \quad n=0, . .,+\infty$ with $\Phi_{n}\left(\overrightarrow{r_{S}}\right)=0$ at the surface of the geometry.
i.e.: $\varphi(\vec{r}, E, t)=\sum_{n=0}^{\infty} \varphi_{n}(E, t) \Phi_{n}(\vec{r})$ and $s(\vec{r}, E, t)=\sum_{n=0}^{\infty} s_{n}(E, t) \Phi_{n}(\vec{r})$

The term $\Phi_{0}(\vec{r})$ is the fundamental mode, and is always positive on the geometry. Hence, every moment of the symmetrized flux satisfies the equation:

$$
\frac{\partial \varphi_{n}(E, t)}{\partial t}=\left\{H_{E}-v D(E) B^{2}\right\}\left[\varphi_{n}(E, t)\right]+s_{n}(E, t)
$$

Assuming that the moments can be factorized in time and space as follows:

$$
\varphi_{n}(E, t)=\sum_{l=0}^{\infty} a_{l, n} \psi_{l}(E) e^{-\lambda_{l} t}
$$

The coefficients $a_{l, n}$ are obtained using a given initial condition. Injecting that expansion in the homogeneous equation without source, we obtain:

$$
-\sum_{l=0}^{\infty} \lambda_{l} a_{l, n} \psi_{l}(E) e^{-\lambda_{l} t}=\sum_{l=0}^{\infty} a_{l, n} e^{-\lambda_{l} t}\left\{H_{E}-v D(E) B^{2}\right\}\left[\psi_{l}(E)\right]
$$

This is possible at any given time $t$ only if:

$$
\left\{H_{E}-v D(E) B^{2}\right\}\left[\psi_{l}(E)\right]+\lambda_{l} \psi_{l}(E)=0
$$

### 10.11.3 Expansion on Eigenfunctions

The expansion of $\varphi_{n}(E, t)$ is valid only if the eigenfunctions $\psi_{l}(E)$ of the Boltzmann operator (without leakage for the time being) form a complete basis. The operator being self-adjoint, these functions form an orthogonal basis, as will be shown in Chap. 12, such that by normalizing them correctly:

$$
\int_{0}^{\infty} \psi_{l}(E) \psi_{l^{\prime}}(E) d E=\delta_{l, l^{\prime}}
$$

M. Ohanian ${ }^{21}$ studied the eigenvalues of the homogeneous and inhomogeneous problem from an analytical and numerical viewpoint. For an infinite medium without leakage, the problem is equivalent to the following eigenvalue problem:

$$
\int_{0}^{\infty}\left\{K\left(E^{\prime} \rightarrow E\right)-v\left(\Sigma_{s}(E)+\Sigma_{a}(E)\right) \delta\left(E-E^{\prime}\right)\right\} \psi_{l}\left(E^{\prime}\right) d E^{\prime}+\lambda_{l} \psi_{l}(E)=0
$$

The particular case of a non-absorbing medium, $\Sigma_{a}(E) \equiv 0$, is simple to study since by the definition of $\Sigma_{s}(E) \equiv \int_{0}^{\infty} \Sigma_{s}\left(E \rightarrow E^{\prime}\right) d E^{\prime}$, we can easily show that the first eigenfunction is equal to $\psi_{0}(E)=\sqrt{m(E)}$. This corresponds to the smallest

[^249]eigenvalue $\lambda_{0}=0$ according to the detailed balance seen in the chapter on thermalization. The eigenvalues are ordered such that $\lambda_{0}<\lambda_{1}<\lambda_{2} \cdots<\lambda_{l}<\lambda_{l+1}<\cdots$. Similarly, if the absorption cross section is inversely proportional to speed, i.e. $\nu \Sigma_{a}(E) \equiv v_{0} \Sigma_{a}\left(E_{0}\right)$ it can be shown that the smallest eigenvalue is $\lambda_{0}=v_{0} \Sigma_{a}\left(E_{0}\right)$ and that $\psi_{0}(E)=\sqrt{m(E)}$ is the associated eigenfunction. Given that the absorption term becomes constant in energy, it can be easily shown that the eigenvalues of the problem with absorption inversely proportional to speed can be deduced from the "zero absorption" case by:
$$
\lambda_{l}=v_{0} \Sigma_{a}\left(E_{0}\right)+\lambda_{l}^{\Sigma_{a}=0}
$$

This implies that the eigenfunctions are the same in both cases. However, in the general case where absorption varies in any way with speed, there is no direct relation with the eigenvalues of the problem without absorption. The Maxwell flux is no longer an eigenfunction of the general problem. If we consider the problem without any absorption, the problem is written under the more convenient form as follows:

$$
\int_{0}^{\infty} K\left(E^{\prime} \rightarrow E\right) \psi_{l}\left(E^{\prime}\right) d E^{\prime}=v \Sigma_{s}(E)-\lambda_{l}^{\Sigma_{a}=0} \psi_{l}(E)
$$

implying an analysis carried out in transport theory by K. M. Case, as explained in Chap. 9. If $\lambda_{l}^{\Sigma_{a}=0} \neq v \Sigma_{s}(E)$ for any energy value, a discrete spectrum of infinite eigenvalues is obtained, associated with a discrete spectrum of eigenfunctions in the conventional framework of the theory of eigenfunctions of an operator. If $\lambda_{l}^{\Sigma_{a}=0}=v \Sigma_{s}(E)$, the RHS can be equal to zero while the LHS is not, thereby leading to a singular behavior of the eigenfunction $\psi_{l}(E)$. Given that the physical quantity $v \Sigma_{s}(E)$ has a minimum value for a minimum energy in the case of a real moderator, as in cases where that quantity increases with energy, any value of $\lambda_{l}^{\Sigma_{a}=0}$ included in the range $\left[\min _{E} v \Sigma_{s}(E),+\infty[\right.$ corresponds to a particular energy $\tilde{E}$ for which $\lambda_{l}^{\Sigma_{a}=0}=v \Sigma_{s}(\tilde{E})$. The value $\lambda_{l}^{\Sigma_{a}=0}=\min _{E} v \Sigma_{s}(E)$ is the limit of the discrete spectrum that defines a maximum order $L$ which is not infinite and thus, cannot lead to a complete basis of eigenfunctions. Consequently, the discrete spectrum of eigenfunctions limited to order $L$ cannot generate a complete basis in the strict mathematical sense, yet, since there exists a continuous spectrum of eigenvalues that depend on energy, the solution including both the discrete and continuous spectrum can be written as:

$$
\varphi_{n}(E, t)=\sum_{l=0}^{L} a_{l, n} \psi_{l}(E) e^{-\lambda_{l} t}+\int_{\min _{E} v \Sigma_{s}(E)}^{+\infty} A_{n}(t, \lambda) \psi(E, \lambda) d \lambda
$$

It is more practical to use the following notation:

$$
\varphi_{n}(E, t)=\sum_{l=0}^{\infty} a_{l, n}(t) \psi_{l}(E)
$$

for which the coefficients $a_{l, n}(t)$ satisfy:

$$
\sum_{l=0}^{\infty} \frac{d a_{l, n}(t)}{d t} \psi_{l}(E)=\sum_{l=0}^{\infty} a_{l, n}(t) \underbrace{H_{E}\left[\psi_{l}(E)\right]}_{-\lambda_{l} \psi_{l}(E)}+s_{l, n}(t) \psi_{l}(E)
$$

i.e.: $\frac{d a_{l, n}(t)}{d t}-\lambda_{l} a_{l, n}(t)=s_{l, n}(t)$
with $s_{l, n}(t) \equiv \int_{0}^{\infty} s_{n}(E, t) \psi_{l}(E) d E$.

### 10.11.4 Case of a Pulsed Source

The case of a pulsed source at time $t_{0}$ as given by $s_{l}(t) \equiv s_{l} \delta\left(t-t_{0}\right)$ leads to $a_{l}(t)=s_{l} e^{-\lambda_{l}\left(t-t_{0}\right)}$, which thus has a symmetrized flux solution:

$$
\varphi(E, t)=\sum_{l=0}^{\infty} s_{l} e^{-\lambda_{l}\left(t-t_{0}\right)} \psi_{l}(E)
$$

For a constant source in time $S(E)$ as from $t_{0}$ (thus forming a Heaviside step function), the response of a pulsed source can be integrated over time:

$$
\varphi(E)=\int_{t=t_{0}}^{+\infty} \varphi(E, t) d t=\sum_{l=0}^{\infty} s_{l} \frac{\psi_{l}(E)}{\lambda_{l}} \text { with } s_{l}=\int_{0}^{\infty} s(E) \psi_{l}(E) d E=\int_{0}^{\infty} \frac{S(E)}{\sqrt{m(E)}} \psi_{l}(E) d E
$$

By reverting back to the flux variable for a pulsed source, and by determining the smallest eigenvalue $\lambda_{0}=v_{0} \Sigma_{a}\left(E_{0}\right)$ for the case of absorption varying with the inverse of speed-corresponding to the Maxwell eigenfunction $\psi_{0}(E)=\sqrt{m(E)}$, we can write:

$$
\Phi(E, t)=a_{0} m(E) e^{-v_{0} \Sigma_{a}\left(E_{0}\right)\left(t-t_{0}\right)}+\sqrt{m(E)} \sum_{l=1}^{\infty} a_{l} \psi_{l}(E) e^{-\left[v_{0} \Sigma_{a}\left(E_{0}\right)+\lambda_{l}^{\Sigma_{a}=0}\right]\left(t-t_{0}\right)}
$$

This demonstrates the asymptotic nature of the Maxwell spectrum as time increases. The case for no absorption ( $v_{0} \Sigma_{a}\left(E_{0}\right) \equiv 0$ ) indeed leads to a Maxwell spectrum that cannot be simplified and that is independent of the detailed form of the slowing-down operator. The latter impacts only the non-zero eigenvalues and their associated eigenfunctions. On the other hand, the case with absorption shows exponential decay of the spectrum; the first term is the longest to decay and is proportional to the Maxwell distribution. If the source is mono-kinetic at energy $E_{0}$ and such that:

$$
s(E, t) \equiv \frac{S(E, t)}{\sqrt{m(E)}} \equiv \frac{S_{0} \delta\left(E-E_{0}\right) \delta\left(t-t_{0}\right)}{\sqrt{m(E)}}
$$

the response to a pulse is written as:

$$
\Phi(E, t)=S_{0} m(E) e^{-v_{0} \Sigma_{a}\left(E_{0}\right)\left(t-t_{0}\right)}+S_{0} \frac{\sqrt{m(E)}}{\sqrt{m\left(E_{0}\right)}} \sum_{l=1}^{\infty} \psi_{l}\left(E_{0}\right) \psi_{l}(E) e^{-\left[v_{0} \Sigma_{a}\left(E_{0}\right)+\lambda_{l}^{\sum_{a}=0}\right]\left(t-t_{0}\right)}
$$

The permanent solution to a constant source in the form of a Heaviside step function of intensity $S_{0} \Theta\left(t-t_{0}\right)$ is written as follows after integration over the range $\left[t_{0},+\infty[\right.$ :

$$
\Phi(E)=\frac{S_{0}}{v_{0} \Sigma_{a}\left(E_{0}\right)} m(E)+S_{0} \frac{\sqrt{m(E)}}{\sqrt{m\left(E_{0}\right)}} \sum_{l=1}^{\infty} \frac{\psi_{l}\left(E_{0}\right) \psi_{l}(E)}{\left[v_{0} \Sigma_{a}\left(E_{0}\right)+\lambda_{l}^{\Sigma_{a}=0}\right]}
$$

For a finite medium, accounting for leakages leads to the operator $\left\{H_{E}-v D(E)\right.$ $\left.B^{2}\right\}[]$, which is self-adjoint but has eigenvalues and eigenfunctions that are different from the operator without leakage $H_{E}[]$, as seen earlier. When the cross section is inversely proportional to speed, the first eigenfunction for a finite medium no longer corresponds to a Maxwell distribution. Given that $\mu_{l}$ and $\varphi_{l}$ are the eigenvalues and eigenfunctions of the operator with leakages, the flux solution is written as follows (similar to calculations carried out earlier):

$$
\Phi(E, t)=\sqrt{m(E)} \sum_{l=0}^{\infty} b_{l} \phi_{l}(E) e^{-\mu_{l}\left(t-t_{0}\right)} \text { with } b_{l} \equiv \int_{0}^{\infty} s(E) \phi_{l}(E) d E
$$

Not only is the permanent asymptotic solution not a Maxwell distribution (as $\phi_{0}$ $(E) \neq \sqrt{m(E)}$, but it also depends on the slowing-down kernel used, through the eigenvalues and eigenfunctions of that kernel. It should be borne in mind that leakages disrupt the equilibrium of the detailed balance, thereby hindering the establishment of a pure Maxwell distribution of neutrons, even when absorption is zero.

### 10.12 Polykinetic Diffusion

All the previous analytical calculations were carried out for monokinetic thermal neutrons or at two energy groups. In a reactor, the real situation is much more complex. If we consider a neutron that is emitted at a given energy, it loses energy by successive collisions. Since the properties of matter depend on energy (namely, the scattering length $L$ and the diffusion coefficient $D$ ), the energy range is discretized to better describe neutron scattering. For a fission reactor, a further difficulty resides in the fact that neutrons are emitted with a fast spectrum. During fission, the energy of neutrons is distributed between 0 and 20 MeV . The fraction of neutrons emitted can be represented by energy groups using several functions. The Watt spectrum models the true spectral distribution of emitted neutrons from fissile nuclides using an empirical mathematical function:

$$
\chi(E)=C e^{-a E} \operatorname{sh} \sqrt{b E}
$$

with: $a=1.012 \mathrm{MeV}^{-1}$ and $b=2.249 \mathrm{MeV}^{-1}$ for the isotope ${ }_{92}^{235} U$. The mean energy of neutrons is given by:

$$
\bar{E}=\frac{\int \chi(E) E d E}{\int \chi(E) d E}=2.01 \mathrm{MeV}
$$

The energy range is discretized in energy groups where the bounds are ( $G$ groups, the index increases with decreasing energy in usual applications):
$E_{\text {fission }}=E_{0}>E_{1}>E_{2}>\ldots>E_{g-1}>E_{g}>\ldots>E_{t h}$ and by defining the characteristics of the material, condensed in energy:

$$
\begin{array}{r}
\Sigma_{g}=\frac{\int_{E_{g}}^{E_{g-1}} \Sigma(E) \Phi(E) d E}{\int_{E_{g}}^{E_{g-1}} \Phi(E) d E} \quad D_{g}=\frac{\int_{E_{g}}^{E_{g-1}} D(E) \Phi(E) d E}{\int_{E_{g}}^{E_{g-1}} \Phi(E) d E} \\
\Sigma_{g \rightarrow g^{\prime}}=\frac{\int_{E_{g}}^{E_{g-1}} d E \int_{E_{g^{\prime}}}^{E_{g^{\prime}-1}} d E^{\prime} \Sigma\left(E \rightarrow E^{\prime}\right) \Phi(E)}{\int_{E_{g}}^{E_{g-1}} \Phi(E) d E}
\end{array}
$$

the $G$ multigroup diffusion equations can be written for a non-multiplying medium as:

$$
-\operatorname{div}\left(D_{g} g r a d \quad \Phi_{g}\right)+\Sigma_{a}^{g} \Phi_{g}+\sum_{g^{\prime} \neq g} \Sigma_{g \rightarrow g^{\prime}} \Phi_{g}=\sum_{g^{\prime} \neq g} \Sigma_{g^{\prime} \rightarrow g} \Phi_{g^{\prime}}
$$

The term $\sum_{g^{\prime} \neq g} \Sigma_{g^{\prime} \rightarrow g} \Phi_{g^{\prime}}$ represents the transfers from faster groups, and eventually from more thermal groups in case of upscattering. For instance, the diffusion equations at 3 energy groups (fast, epithermal, thermal with upscattering towards the epithermal group), are written as:

$$
\left.\begin{array}{c}
\Delta \Phi_{1}-\frac{1}{L_{1}^{2}} \Phi_{1}=0 \\
\Delta \Phi_{2}-\frac{1}{L_{2}^{2}} \Phi_{2}=-\frac{1}{L_{1 \rightarrow 2}^{2}} \Phi_{1}-\frac{1}{L_{3 \rightarrow 2}^{2}} \Phi_{3} \\
\Delta \Phi_{3}-\frac{1}{L_{3}^{2}} \Phi_{3}=-\frac{1}{L_{1 \rightarrow 3}^{2}} \Phi_{1}-\frac{1}{L_{2 \rightarrow 3}^{2}} \Phi_{2}
\end{array}\right\} \begin{gathered}
L_{1}^{2}=\frac{D_{1}}{\Sigma_{t 1}} \\
\text { with }\left\{\begin{array}{c}
D_{2}=\frac{D_{2}}{\Sigma_{t 2}}, L_{1 \rightarrow 2}^{2}=\frac{D_{2}}{\Sigma_{1 \rightarrow 2}}, L_{3 \rightarrow 2}^{2}=\frac{D_{2}}{\Sigma_{3 \rightarrow 2}} \\
L_{3}^{2}=\frac{D_{3}}{\Sigma_{t 3}}, \quad L_{1 \rightarrow 3}^{2}=\frac{D_{3}}{\Sigma_{1 \rightarrow 3}}, \quad L_{2 \rightarrow 3}^{2}=\frac{D_{3}}{\Sigma_{2 \rightarrow 3}}
\end{array}\right.
\end{gathered}
$$

Calculation of the neutron constants of materials condensed in energy depends on the energy variation of the properties as well as the neutron spectrum $\Phi(E)$. These diffusion constants can be obtained either by experimental measurements as discussed in the previous paragraph or by calculation from numerical simulations dealing with neutron transport in different materials. For example, we can calculate the fast [ $20 \mathrm{MeV}, 1 \mathrm{MeV}$ ], epithermal [ $1 \mathrm{MeV}, 0.4 \mathrm{eV}$ ] and thermal [ 0.4 eV , $10^{-11} \mathrm{MeV}$ ] flux resulting from the attenuation of a beam of monokinetic neutrons in a slab of water, steel or concrete (at 2 MeV for our case ${ }^{22}$ ) as computed by the Monte Carlo method. A source of 1000 neutrons per second is imposed in a cubic driver zone called the "fuel" that feeds neutrons to a scattering medium along the $x$ axis, and for which we compute the attenuation properties. The reflective conditions imposed on the boundaries of the pattern (except for the edge where there is vacuum) leads to a calculation representative of an infinite medium (Figs. 10.32 and 10.33).


Fig. 10.32 Numerical modeling of the attenuation in a scattering medium

[^250]

Fig. 10.33 Attenuation of 2 MeV neutrons in water (blue), in concrete (purple) and in steel (black) [the $x$-axis is the penetration depth in cm and the $y$-axis is the thermal flux in $\mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}$ ]

If it were a surface source, the theoretical net fast current obtained ( $J_{1}>1 \mathrm{MeV}$ ) would be $\frac{1000 \text { neutrons of } 2 \mathrm{MeV} / \mathrm{s}}{100 \mathrm{~cm}^{2}}=10 \mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}$. In our case, the reflective conditions around a cubic source result in a source/medium interface through which a net current of 1000 neutrons per second passes, and in the existence of a
non-zero current from the medium to the source. The current from the source to the medium is hence 1000 neutrons/s larger than the inverse current, the net current being equal to $J=J^{-}-J^{+}$. This effect is due to the back-scattering (reflector effect) of some fast neutrons that are slowed down with heavy nuclides but are not absorbed. It may be observed that the fast flux is rapidly attenuated by an exponential decay that depends on the penetration depth, thus being consistent with the diffusion theory (with the flux having the form of $\Phi_{1}(x)=\Phi_{1}(0) e^{-x / L_{1}}$ ). As steel is a poor moderator, the epithermal flux is larger than that in water, which slows down neutrons efficiently, and that in concrete, which also contains water. Neutrons, slowed down by the hydrogen in water, lose almost all their energy, and in some very rare cases, end up in the thermal domain without passing through the epithermal energy domain. It is clear that the rise in thermal flux is very apparent in the cases of water and concrete. Thermal neutrons are almost completely absorbed by steel, which is a very efficient thermal absorbing material used in the control rods of PWR, and in the barrel of the EPR to protect the vessel. Due to the high atomic mass of its constituent atoms, steel is less efficient than water (which contains hydrogen that is a very good moderator) in attenuating fast neutrons, but the successive layers of water (that efficiently thermalize fast neutrons) and steel (that efficiently absorbs thermal neutrons, thermalized by the water used as a shield) ensure global protection. Finally, it should be noted that the epithermal and thermal flux are greater than the fast flux that induced their emission, since there is a neutron concentration at low energies which accumulates until they disappear by thermal absorption.

The choice of using monokinetic neutrons at the mean energy of the fission spectrum leads to a bias with respect to the true Watt spectrum, which modifies the global attenuation of fast neutrons.

Numerical neutron shooting experiments in moderators simulate experiments in piles that attenuate neutrons without being hindered by radial leakages, given that reflective boundary conditions are applied at the interface. It should be noted that the radial leakages of a non-reflective pile with zero-flux at the exterior radial surface (such as the previously described Marius experiment) are characterized by buckling $2(\pi / a)^{2}$. The smaller the pile, the greater the buckling, which strongly impacts the measurements. However, the difficulty in modeling is due to the fact that the group-wise fluxes are highly perturbed by subsequent increases in energy of the neutrons by thermalization close to the source, rendering calculation of attenuation coefficients by scattering prone to uncertainties. These flux variations (for instance thermal flux) are very abrupt on small layers. Besides, they do not exhibit exponential behavior, whence the difficulty of assimilating them in the absence of a very fine spatial solution.

Figure 10.34 shows the impact of the neutron spectrum (injection of monokinetic neutrons of 2 MeV in the first case, and that due to the Watt spectrum in the second case) on attenuation and the difficulty in defining the appropriate scattering lengths. Regression calculation on the first 5 centimeters, and applied to the fast flux, leads to discrepancies of more than $50 \%$ on $L_{1}$. This type of analysis, where the interface effects are neglected, nonetheless leads to computation of the attenuation coefficients (in $\mathrm{cm}^{-1}$ ) or scattering lengths (the inverse of the


Fig. 10.34 Effect of neutron energy on attenuation in water

Table 10.2 Fast diffusion length $L_{1}$ for various materials in contact with a source of uranium 235

| $L_{1}[\mathrm{~cm}]$ for each material | Neutrons of 2 MeV | Watt neutrons |
| :--- | :--- | :--- |
| Pure steel | 6.7 | 7.0 |
| Stainless steel | 6.5 | 6.8 |
| Concrete | 7.2 | 10.7 |
| Light water | 4 | 7 |
| Graphite | 7.8 | 11.8 |
| Heavy water | 4.6 | 7.7 |
| Heat conductor | 161.3 | 153.8 |

Table 10.3 Epithermal diffusion length $L_{2}$ for various materials

| $L_{2}[\mathrm{~cm}]$ | 0.2 MeV | 0.4 MeV | 1 MeV | 2 MeV | Watt |
| :--- | :--- | :--- | :--- | :--- | ---: |
| Pure steel | 21.5 | 26.4 | 29.1 | 31.8 | 30.2 |
| Stainless steel | 15.2 | 19.0 | 22.9 | 24.7 | 23.2 |
| Concrete | 5.0 | 5.1 | 5.8 | 7.8 | 10.5 |
| Light water | 1.5 | 1.8 | 2.6 | 4.1 | 6.2 |
| Graphite | 6.4 | 6.6 | 7.2 | 8.9 | 11.3 |
| Heavy water | 5.6 | 5.7 | 5.8 | 6.1 | 6.9 |

attenuation coefficient) that are particularly useful for fluence subjects or radioprotection (Tables 10.2 and 10.3).

The scattering lengths at 3 energy groups (Table 10.4) show that concrete behaves like low-density water towards neutrons. The other isotopes in concrete are quite inefficient in slowing down neutrons. Graphite and heavy water, with low absorption that allows for high values of thermal scattering lengths (more than 50 cm ), behave as "ideal moderators". In homogeneous problems, without neutron guides, these values of the scattering lengths entail calculations of the same order of magnitude as the attenuated flux, which are realistic. The attenuation problems in

Table 10.4 Thermal diffusion length $L_{3}$ for various materials

| $L_{3}[\mathrm{~cm}]$ | 0.2 MeV | 0.4 MeV | 1 MeV | 2 MeV | Watt |
| :--- | :--- | :--- | :--- | :--- | ---: |
| Concrete | 9.6 | 9.6 | 9.9 | 10.5 | 11.4 |
| Light water | 2.8 | 2.9 | 3.2 | 4.3 | 6.0 |
| Graphite | 53.8 | 53.8 | 54 | 54.6 | 11.3 |
| Heavy water | 96.2 | 96.2 | 96.2 | 96.2 | 94.3 |

concrete are central to the question of decommissioning of nuclear reactors. Indeed, some fast neutrons may propagate very far in the core, especially if they are favored by neutron guides, i.e. slices or paths oriented towards the reactors, and necessary for introducing the instrumentation in the core for instance. Besides, these neutron guides may propagate neutrons over structures comprising steel that contains cobalt, which produces redoubtable ${ }^{60} \mathrm{Co}$ through radioactivity. In addition, through neutron activation, cobalt creates the gamma $\gamma$ radiation that constitutes one of the principal sources of dose effects in radioprotection. At such distances from the core, deterministic calculations are not sufficiently precise and may even be inefficient. In the end, only Monte Carlo calculations with large number of particles can give an idea of geometrical and point-wise effects.

## Chapter 11 <br> Nuclear Reactor Reactivity

The reactivity of the core is the most global parameter that helps to understand the behavior of a reactor. The precise calculation of core reactivity is the major concern of neutron physicists and engineers and the branch of physics that deals with it must be well understood. Defining it is not as easy as it may initially seem.

### 11.1 Multiplication Factor of a Chain Reaction

### 11.1.1 Deterministic Approach to Chain Reactions

For a neutron emitted by fission, $\alpha$ is the probability that it will penetrate the new fissile nuclide. Given that $v$ is the mean number of neutrons generated by fission, some of these undergo sterile capture, for instance radiative capture $(n, \gamma)$ on the ${ }_{92}^{238} U$ isotope. Finally, for each absorbed neutron, there will be $\eta=\nu \sigma_{f} /\left(\sigma_{f}+\sigma_{c}\right)$ new neutrons since the probability of the nuclide fissioning is $\alpha=\sigma_{f} /\left(\sigma_{f}+\sigma_{c}\right) . \eta$ is the number of neutrons produced per absorbed neutron. It is thus inherently smaller than $v$. The effective multiplication factor ( $k_{\text {eff, }}$, pronounced " $k$ effective") is the product of the probability of the number of neutrons emitted by absorption by the probability of them penetrating the nuclide, i.e. $k_{\text {eff }}=\alpha \eta$. By its very definition, the neutron population changes as a geometric progression of common ratio $k_{\text {eff }}$ :


If $k_{\text {eff }}$ is greater than one, the multiplication reaction increases rapidly and the reactor is said to be over-critical. The more $k_{\text {eff }}$ exceeds 1, the greater the increase in the nuclear power. If $k_{\text {eff }}$ is far larger than 1, nuclear explosion occurs (keeping in
mind that $k_{\text {eff }}$ cannot be greater than $v$, the average number of neutrons produced by fission). Ultimately, the temperature increase deforms the fissile medium and the loss of geometry arrests the phenomenon. Where $k_{\text {eff }}$ is less than 1 , the reaction is "choked" and the reactor is said to be subcritical and the neutron population tends to 0 . If $k_{e f f}$ is strictly equal to 1 , the neutron population is stable: the reactor is critical. The term "critical" has a precise meaning in this context but may be misunderstood by the layman, for whom it normally signals danger. It must therefore be used with care in non-specialist discussions. By definition $k_{\text {eff }}$ is dimensionless. Neutron physicists use a quantity derived from $k_{\text {eff }}$ known as reactivity; it is always denoted by the Greek letter $\rho$ and is computed as follows:

$$
\begin{equation*}
\text { Definition of reactivity: } \quad \rho_{[-]} \equiv \frac{k_{e f f}-1}{k_{e f f}} \tag{11.1}
\end{equation*}
$$

In practice, reactivity is far less than 1 and is quantified in per cent mille [hundred-thousandths] ( $1 \mathrm{pcm}=10^{-5}{ }_{[-]}$). Use of the criterion expressing $k_{\text {eff }}$ in relation to 1 appears an extremely mathematical approach, and one might well wonder how an actual reactor may be built such that its $k_{\text {eff }}$ is exactly equal to 1. Nevertheless, as we will see, variation in this parameter can be very small in terms of the reasonable variation of physical parameters; in other words, reasonable variation in $k_{\text {eff }}$ results in slow and controllable variation in the physical parameters. The meanings of criticality and multiplicity must be clearly distinguished. A physical medium is said to be under-multiplying/over-multiplying if the number $c$ of secondary neutrons produced by a neutron-nuclide collision is smaller/greater than one respectively for all collision points and for all speeds of the incident neutron. Physically, an under-multiplying medium cannot ensure that a chain reaction is maintained. In a self-multiplying medium (i.e. the number of neutrons produced is equal to 1 ), leakage within the system may be expected to hinder a permanent chain reaction. These results can be demonstrated mathematically in transport theory. The mathematical work of P. Nelson (Fitzgibbon and Walker 1977, p. 173) showed that in diffusion theory, an under-multiplying homogeneous medium induces subcriticality, although there are not as yet any firm conclusions regarding the case of a self-multiplying medium.

### 11.1.2 Stochastic Approach to Chain Reaction

In the previous approach, it was assumed that the number of neutrons emitted by fission was constant between each generation $(=\bar{v})$. In reality, the phenomenon is more complex: the integer number $v$ ranges between 1 and 6 , creating fluctuation over generations. This stochastic model of the transport equation and its impact on neutron kinetics have been studied by various authors since the 1960s, including

Austin Blaquière and Victor Raïevski in France, and more recently, Richard Sanchez, ${ }^{1}$ whose works are summarized here for an infinite medium.


Richard Sanchez (circa 2005) (Courtesy Sanchez)
The probability of obtaining $m$ neutrons after $g$ generations, assuming a starting figure of $n$, is expressed as $P_{n, m}(g)$. To compute the extinction probability $q$ of a chain reaction associated with a given neutron, it must be noted that the probability of neutron capture is $P_{1,0}(1)$, and that neutrons can generate either one (in the case of fission that rarely emits one neutron) or several particles (in conventional fission where several neutrons are emitted) with a probability of $P_{1, m}(1)$, and so on in a chain reaction.

[^251]Hence, the probability $P_{2,2}(1)$ represents the behavior of two initial neutrons and two processes may be involved:

- either one of the two initial particles is absorbed and the other produces two neutrons by fission (two symmetrical processes),
- or each neutron produces one neutron after fission.
$q$ is therefore characterized by the Hansen ${ }^{2}$ equation:
Hansen equation: $\quad q=P_{1,0}(1)+\sum_{m>0} P_{1, m}(1) \quad q^{m}=\sum_{m \geq 0} P_{1, m}(1) \quad q^{m} \equiv G(q)$

Mathematical analysis of the function $G(x)$ shows that it is always equal to 1 for $x=1$ and its derivative at that point, $d G(x) /\left.d x\right|_{1}=\sum_{m \geq 0} m P_{1, m}(1)=\bar{m}$, is equal to the mean number of neutrons per generation. ${ }^{3}$

Physically, the extinction probability may be expected to be smaller than 1 where $\bar{m}>1$, and even equal to zero, but the realistic plot from Fig. 11.1 shows that this is not the case. The probabilities $P_{n, m}(g)$ may be computed sequentially, since ongoing events are in fact independent of past events (captures do not modify the cross sections of the material being considered):

$$
\left\{\begin{array} { l } 
{ P _ { n , m } ( g + g ^ { \prime } ) = \sum _ { k \geq 0 } P _ { n , k } ( g ) P _ { k , m } ( g ^ { \prime } ) } \\
{ P _ { n + n ^ { \prime } , m } ( g ) = \sum _ { m ^ { \prime } = 0 } ^ { m ^ { \prime } = m } P _ { n ^ { \prime } , m ^ { \prime } } ( g ) P _ { n , m - m ^ { \prime } } ( g ) }
\end{array} \text { and } \left\{\begin{array}{l}
P_{0, m}(g)=\delta_{0, m} \\
P_{n, m}(0)=\delta_{n, m}
\end{array}\right.\right.
$$

These formulae are used to calculate in a recursive manner all the probabilities as a function of the basic probabilities after one generation $P_{1, m}(1)$. These probabilities depend on the cross sections of the materials in which the neutrons exist. $G$ (x) may be extended:

[^252]Fig. 11.1 Generating function $G(x)$ (after R. Sanchez)


$$
G_{n}(g, x) \equiv \sum_{m \geq 0} P_{n, m}(g) x^{m}
$$

and satisfies the following recurrence relations:

$$
\left\{\begin{array} { l } 
{ G _ { n + n ^ { \prime } } ( g , x ) = G _ { n } ( g , x ) G _ { n ^ { \prime } } ( g , x ) } \\
{ G _ { n } ( g + g ^ { \prime } , x ) = G _ { n } ( g , G _ { 1 } ( g ^ { \prime } , x ) ) }
\end{array} \quad \text { and } \quad \left\{\begin{array}{l}
G_{0}(g, x)=1 \\
G_{n}(0, x)=x^{n}
\end{array}\right.\right.
$$

thus: $G_{1}(g, x)=G o G o \ldots \ldots$ o $G(x) \equiv G^{g}(x) \quad$ and $\quad G_{n}(g, x)=\left(G_{n}(g, x)\right)^{n}$
The extinction probability $q_{n}(g)=G_{n}(g, 0)$ associated with the probabilities $P_{n, m}(g)$ thus verifies that $q_{n}(g)=\left[q_{1}(g)\right]^{n}$ and $q_{1}(g)=G\left(q_{1}(g-1)\right)=\ldots=G^{n}\left(\delta_{n, 0}\right)$. Hence:

$$
q=\lim _{g \rightarrow \infty} q_{1}(g)=\lim _{g \rightarrow \infty} G^{g}(0)=G^{\infty}(0)
$$

The value of $G^{\infty}(0)$ is obtained by a fixed point iteration on the equation $G(x)=$ $x$ and leads to the smallest root of Fig. 11.1. If $\bar{m}>1$, the chain reaction dies out with a non-zero probability. If $\bar{m} \leq 1$, the chain reaction dies out in a finite number of generations with a probability of $G^{\infty}(0)=1$, i.e. with certainty. The mean number of neutrons at generation $g$ and the variance thereof are given by:

$$
\left\{\begin{array}{l}
N_{n}(g)=n N_{1}(g)=n \bar{m}^{g} \\
{\left[\sigma_{n}(g)\right]^{2}=n\left[\sigma_{1}(g)\right]^{2}=n \sigma^{2} \bar{m}^{g-1} \bar{m}^{g}-1} \\
\bar{m}-1
\end{array}\right.
$$

These results follow from the fact that as regards the mean and variance associated with $G_{n}(g, x)$, the mean of a sum of random variables is equal to the sum of the mean values, and similarly, the variance of a sum of independent random
variables is equal to the sum of variances. Further, for a mean random variable $m$ of variance $\sigma^{2}$ and of generating function $G(x)$, we obtain:

$$
\bar{m}=G^{\prime}(1), \quad \sigma^{2}=G^{\prime \prime}(1)-\bar{m}(\bar{m}-1)
$$

Since $G_{1}(g, x)=G^{g}(x)$, the following recurrence relations are obtained:

$$
N_{1}(g)=\bar{m} N_{1}(g-1), \quad \sigma_{1}^{2}(g)=\bar{m}^{2} \sigma_{1}^{2}(g-1)+\sigma^{2} \overline{m^{g}-1}
$$

The reduced variance is: $\left[\widehat{\sigma}_{n}(g)\right]^{2}=\frac{\left[\sigma_{n}(g)\right]^{2}}{\left[N_{n}(g)\right]^{2}}=\frac{\sigma^{2}}{n} \frac{1-\bar{m}^{-g}}{\bar{m}(\bar{m}-1)}$
Sanchez points out the seemingly astonishing fact that an infinite selfmultiplying system ( $\bar{m}=1$ ) cannot maintain a chain reaction indefinitely, which is unusual since the limit $\lim _{g \rightarrow \infty} N_{n}(g)=n$ becomes constant between two generations. However, while the probability of an infinite chain reaction is zero, the number of neutrons in that chain tends to infinity, as well as reduced variance, thus removing any contradiction. A further surprising fact is that even in an overmultiplying system, there is a non-zero probability of the reaction dying out for a small number of neutrons probably after few generations, due to the variability of the number of neutrons emitted by fission. However, this result is not obtained if this number is taken to be constant $(=\bar{v})$ in the classical deterministic approach, although increase in a significant population cannot be stopped solely by statistical considerations. Furthermore, we must consider that all states having a finite number $m$ of neutrons may only be transients, since according to Markovian analysis, they can appear only a finite number of times. Consequently, the probability of such a state tends to zero when the number of generations tends to infinity, regardless of the value of $\bar{m}$. Hence, for $\bar{m}>1$, either the chain can die out statistically for a small number of neutrons or the system tends to infinity as predicted by the deterministic analysis. The possible use of this statistical approach will be discussed later with regard to neutron noise analysis (Table 11.1).

Table 11.1 Asymptotic behavior of a chain reaction

| $\bar{m}$ | $\lim _{g \rightarrow \infty} N_{n}(g)$ | $\lim _{g \rightarrow \infty}\left[\widehat{\sigma}_{n}(g)\right]^{2}$ | $\lim _{g \rightarrow \infty} q_{n}(g)$ |  |
| :--- | :--- | :--- | :--- | :--- |
| $\bar{m}>1$ | $\infty$ | $\frac{\sigma^{2}}{n_{m}} \frac{1}{\overline{(m-1)}}$ | $<1$ | Either the chain reactions die out after some <br> generations or they tend to infinity |
| $\bar{m}=1$ | $n$ constant | $\infty$ | 1 | As above, but the probability of diverging <br> chains tends to 0. The reduced variance <br> increases linearly with the number of gener- <br> ations and tends to infinity |
| $\bar{m}<1$ | $\infty$ | $\infty$ | 1 | All chain reactions die out after a finite <br> number of generations |



Fig. 11.2 The neutron life cycle

## 11.2 "Four-factor" Formula

The four-factor formula is a mnemonic calculation method in physics and is of significant historical interest since it was used to calculate the Fermi pile by careful evaluation of each factor without discounting the leakage term, as will be discussed.

The neutron life cycle is shown in Fig. 11.2 where for an absorbed neutron, the following are quantified:

- excess neutrons provided by fast fission $(\varepsilon)$,
- leakage during slowing-down (non-leakage probability $P_{r}$ ),
- neutrons lost in the resonant captures (escape probability $p$ ),
- leakage in the thermal domain (non-leakage probability $P_{t h}$ )
- sterile captures (thermal utilization factor $f$ ).

For an infinite reactor without leakage, the non-leakage probabilities are equal to $1\left(P_{r}=P_{\text {th }}=1\right)$, and thus the "four-factor" formula is obtained and $k_{e f f}$ is named $k_{\infty}$ ( $k$ infinite) (Etherington 1957, pp. 6-121):

$$
\begin{equation*}
\text { Four-factor formula: } \quad k_{\infty}=\eta \varepsilon p f \tag{11.3}
\end{equation*}
$$

If $k_{\text {eff }}<1$ (subcritical), the neutron population may be kept stable by introducing a source $S$ (neutrons $/ s$ ). If $\ell$ is the neutron lifetime, i.e. $S \ell$ is the mean number of neutrons produced in the medium over time $\ell$, at the second generation, after time $\ell$,


Fig. 11.3 Neutron multiplication in a subcritical state with a source
there will be $k_{\text {eff }} S \ell$ neutrons, by the very definition of $k_{\text {eff. }}$. Over the same time period, $S$ $\ell$ new neutrons will be produced, and so on, as depicted in Fig. 11.3:

The number of neutrons present in the medium after an infinite number of generations is thus given by (Bonilla 1957, p. 171):

$$
n_{\text {total }}=S \ell\left(1+k_{e f f}+k_{e f f}^{2}+\cdots+k_{e f f}^{n}+\cdots\right)=\frac{S \ell}{1-k_{e f f}}
$$

Hence the flux level is proportional to the source intensity. This situation occurs in a power reactor in which to start-up the core, a primary ${ }_{98}^{252} C f$ source is introduced (and subsequently removed) and secondary sources are used. It should be noted that the previous formula has no meaning for a critical reactor in which an independent source cannot induce a permanent regime.

### 11.2.1 Detailed Analysis of the Four-factor Formula

With the four-factor formula, the multiplication factor can be written as a function of four quantities that are representative of the fuel: $\eta, \varepsilon, p$ and $f$. Some authors ${ }^{4}$ represent neutron production schematically in a highly didactic fashion, adding an energy dimension, for better understanding the four-factor formula. The x-axis in this scheme represents successive generations of neutrons over time while the $y$-axis corresponds to the energy of the neutrons, with the behavior of the latter simplified by assuming that absorptions occur only at thermal energy and that fissions produce mono-energy neutrons at energy $E_{0}$. The four-factor formula idealizes the behavior of neutrons by limiting the possibilities of interaction with matter in specific energy domains (Bonilla 1957, p. 173) (Fig. 11.4).

[^253]Fig. 11.4 The four-factor formula represented with an energy scheme


Table 11.2 Mean number of neutrons and fuel multiplication factor for major fissile isotopes

|  | $v$ | $\eta$ |
| :--- | :--- | :--- |
| ${ }_{92}^{233} U$ | 2.55 | 2.29 |
| ${ }_{92}^{235} U$ | 2.47 | 2.09 |
| ${ }_{92}^{238} U$ | 2.56 | 0 |
| ${ }_{92}^{239} \mathrm{Pu}$ | 2.91 | 2.10 |

Table 11.3 The fuel multiplication factor as a function of fuel enrichment

| ${ }_{92}^{235} U / U_{\text {total }}(\%)$ | $\eta$ |
| :--- | :--- |
| 0.71 (natural uranium) | 1.34 |
| 1.4 | 1.60 |
| 5 | 1.88 |
| 20 | 2.08 |
| 100 | 2.09 |

### 11.2.1.1 Fuel Multiplication Factor $\boldsymbol{\eta}$

When a neutron causes a fission, $v$ neutrons are emitted on average (Table 11.2). However, when a neutron is absorbed at the thermal energy, it does not necessarily induce a fission reaction since it has a given probability of causing a $(n, \gamma)$ reaction. The relevant quantity is thus the number of neutrons emitted per neutron absorbed in the fuel. This number, $\eta$, is the fuel multiplication factor. If $\Sigma_{a}$ and $\Sigma_{f}$ are respectively the absorption and fission cross sections of the fuel, $\eta=\nu \Sigma_{f} / \Sigma_{a}$. Recall that $\Sigma_{a}=\Sigma_{f}+\Sigma_{c}$.

In a thermal reactor, the fissile isotope (e.g. ${ }_{92}^{235} U$ ) is generally associated with a non-fissile isotope (in thermal, e.g. ${ }_{92}^{238} U$ that is fertile), and $\eta$ is then obtained by weighing the respective fission rates of the $\eta$ values of the fissile isotopes in the fuel. $\eta$ can be computed as a function of ${ }_{92}^{235} U$ enrichment.

Table 11.3 shows that $\eta-1$, which is the number of excess neutrons in relation to the neutron needed to maintain the chain reaction, increases with enrichment. $\eta$ depends significantly on the incident neutron energy: the plot of $\eta$ for the isotopes ${ }_{92}^{235} U,{ }_{92}^{238} U$ and ${ }_{94}^{239} P u$ illustrates this phenomenon (cf. Figs. 11.5, 11.6 and 11.7). In particular, it can be seen that $\eta$ is equal to 0 for the ${ }_{92}^{238} U$ isotope up to a given threshold of 1 MeV , since this isotope is fissile only at fast energies (despite having
a non-zero value of $v$, which does not impact the fission reaction rate since the cross section of ${ }_{92}^{238} U$ is very small and below 2 MeV ).

Further, at high energies, $\eta$ and $v$ are equal to one another due to the fact that the capture cross section becomes negligible at high energy even if it no longer has an inverse-speed law variation (which is generally applied at low at intermediate energies). To optimize the number of neutrons generated, it is best to have a fast spectrum: high value of $\eta$ and small capture cross sections as well as ${ }_{92}^{238} U$ which becomes fissile.

For a mixture of isotopes, the fuel multiplication factor is given by the formula:

$$
\eta=\frac{\sum_{i \in f u e l} v_{i} \Sigma_{f}^{i}}{\sum_{i \in f u e l} \Sigma_{a}^{i}}=\sum_{i \in f u e l} \eta_{i} \frac{\Sigma_{a}^{i}}{\sum_{i \in f u e l} \Sigma_{a}^{i}}
$$

This parameter, which naturally depends on the incident neutron energy, is equal to 2 at low energy and increases as of 0.1 MeV to values approaching 4 at 10 MeV .

U235 from JEFF 3.0 from Local


Fig. $11.5 \eta$ (dark) and $\nu$ (light) for ${ }_{92}^{235} U$ (from JEFF 3.0)


Fig. 11.6 $\eta$ (dark) and $v$ (light) pour ${ }_{92}^{238} U$ (from JEFF 3.0)

### 11.2.1.2 Fast Fission Factor $\varepsilon$

Fission neutrons can cause another fission immediately even before slowing down. However, in a thermal reactor, this effect is small. Nevertheless, it must be taken into account by considering that $\eta \varepsilon$ fast neutrons are available per neutron captured in the fuel. $\varepsilon$ is the fast fission factor of the order of 1.03-1.04 for standard reactors using natural uranium (Fig. 11.8).

At the temperatures encountered in pressurized water reactors, $\varepsilon$ is almost independent of temperature. It depends solely on the radius of the fuel and the amount of ${ }_{92}^{238} U$ that can be considered as being constant since it is the most abundant isotope in the fuel. (Bennet 1981, p. 81) proposes the following correlation, valid for water-moderated reactors with enriched fuel:
in which [] represents the concentration.

Pu239 from JEFF 3.0 from Local


Fig. $11.7 \eta$ (red) and $v$ (green) for ${ }_{94}^{239} P u$ (from JEFF 3.0)


Fig. 11.8 Effect of radius of a natural uranium rod on the fast fission factor [after (Kahan and Gauzit 1957)]

### 11.2.1.3 Neutron Slowing-down: Escape Probability Factor

The neutrons are slowed down by inelastic collisions at high energy then by elastic collision on light nuclides ( $H, D, B e$ or $C$ ) in the moderator. At high energies, capture by materials used in the nuclear reactor (fuel cladding, various structures) is negligible. However, when neutrons are slowed down to energies of a few tens of electronVolts, they reach the region in which capture resonances or traps are present, if the medium contains a resonant absorbing isotope such as ${ }_{92}^{238} U$ or ${ }_{90}^{232} T h$. If we define $p$ as the probability of escaping resonant capture, there are
only $\eta \varepsilon p$ neutrons available in the thermal energy range per neutron absorbed in the fuel. In a reactor with uranium $3.2 \%$ enriched with ${ }_{92}^{235} U, p$ is of the order of 0.7. $p$ can be calculated analytically under some simplifying assumptions as seen previously. It contains the resonance integral of the resonant isotope.

### 11.2.1.4 Thermal Range: The Thermal Utilization Factor

(Bonilla 1957, p. 207)
In the thermal energy range, the absorption (capture + fission) cross section of the fuel is very large, but the absorption cross sections of the moderator and structure materials (zirconium cladding, boron in water, assembly grids) are not negligible ( $1 / v$ law). There is competition between useful absorption in the fuel and parasitic capture in other materials. $f$ is defined as the thermal utilization factor, the ratio between the number of neutrons absorbed in the fuel and the total number of neutrons absorbed. If $\Phi_{\text {fuel }}, \Phi_{\text {mod }}$ and $\Phi_{\text {structure }}$ are the mean thermal flux in the fuel, moderator and different materials (cladding, guides, plugs, etc.) respectively; $\sigma_{a}^{\text {fuel }}$, $\sigma_{a}^{\bmod }$ and $\sigma_{a}^{\text {structure }}$ the microscopic absorption cross sections; $N_{f u e l}, N_{\text {mod }}$ and $N_{\text {structure }}$ the number of nuclides per $\mathrm{cm}^{3} ; V_{\text {fuel }}, V_{\text {mod }}$ and $V_{\text {structure }}$ the volumes of these different materials:

$$
f=\frac{N_{\text {fuel }} \sigma_{a}^{\text {fuel }} V_{\text {fuel }} \Phi_{\text {fuel }}}{N_{\text {fuel }} \sigma_{a}^{\text {fuel }} V_{\text {fuel }} \Phi_{\text {fuel }}+N_{\mathrm{mod}} \sigma_{a}^{\bmod } V_{\bmod } \Phi_{\mathrm{mod}}+\sum_{\text {structures }} N_{\text {structure }} \sigma_{a}^{\text {structure }} V_{\text {structure }} \Phi_{\text {structure }}}
$$

Finally, for each thermal neutron absorbed in the fuel, after each complete cycle, $\eta \varepsilon p f=k_{\infty}$ neutrons are available for absorption at the next cycle. If $k_{\infty}$, the global multiplication factor in infinite medium, is greater than or equal to 1 , it is possible to maintain a chain reaction in such a medium assumed to be infinite (if $k_{\infty}>1$, it is divergent, and if $k_{\infty}=1$, it is self-supporting). For a true set-up with finite dimensions, it is necessary that $k_{\infty}>1$ to compensate for neutron leakage from the reactor volume, and more commonly, to compensate for the creation of absorbing fission products in order to produce energy for an industrially viable period.

### 11.2.2 Technological Moderation Ratio Effect on the Fourfactor Formula

The technological moderation ratio is defined as the ratio of moderator volume (which quantifies moderation) to the fuel volume (which quantifies the ability to generate neutrons). Variation in $k_{\infty}$ can be plotted in relation to this ratio as shown in Fig. 11.9. It may be seen that the escape probability factor $p$ tends towards 1 as the moderation ratio tends towards infinity. This means that if the moderator volume increases indefinitely, or the fuel volume tends towards 0 , the neutron is no longer able to interact geometrically with the fuel and be captured by


Fig. 11.9 Variation of the multiplication factor with the moderation ratio
it. According to the same logic, the thermal utilization factor $f$ tends towards 0 under the same conditions. For a given fuel, $\eta$ and $\varepsilon$ may be considered almost constant (however, this reasoning has its limits when moderation tends towards 0 or infinity, although such cases have no practical applications!). As a function of the moderation ratio, $k_{\infty}$ has a maximum value, which for pressurized water reactors is around 4. Reactor designers seek to attain this optimal level to the utmost since it is the value that allows maximum utilization of the expensive fuel when in the core.

### 11.3 Allowing for Leakages in a Finite Reactor

Leakage occurs in finite reactors due to neutrons that travel out of the reactor by scattering without being absorbed. If no reflector directs these neutrons back towards the core, they are lost for the chain reaction. The scheme shown previously helps account for this phenomenon (Fig. 11.10) via non-leakage probabilities in the fast $\left(P_{r}\right)$ and thermal $\left(P_{t h}\right)$ energy domains. It should be noted that a scheme using two energy groups (fast and thermal) is commonly used, but that this may be extended to several groups.

The above diagram contains non-leakage probabilities for the geometrical domain of the reactor. In two-group theory, these probabilities are given as follows. $P_{r}=1 /\left(1+L_{r}^{2} B^{2}\right)$ is the non-leakage probability of the neutron during its slowingdown until it reaches the thermal group cut-down, $L_{r}$ being the diffusion length integrated over the fast group. $P_{t h}=1 /\left(1+L_{t h}{ }^{2} B\right)$ is the non-leakage probability of


Fig. 11.10 Determining leakage in a finite reactor
the neutron in the thermal group, with $L_{t h}$ being the scattering length integrated over the thermal group. The quantity $L_{t h}$ should not be confused with the classical diffusion length $L$, which is valid for neutrons that are completely thermalized (at 0.0253 eV ). $L_{\text {th }}^{2}$ corresponds rather to a migration area averaged over the thermal group only. Fermi's age theory, which will be discussed below, can be used to calculate the non-leakage probabilities $P_{r}$ and $P_{t h}$. In a $P W R$, the fast non-leakage probability $P_{r}$ is around 0.97 and the thermal non-leakage probability, $P_{t h}$, is around 0.99 .

### 11.4 Two-group Multiplication Factor

When knowledge of cross sections was sufficiently advanced, physicists rendered flux calculation in the reactor more complex using a two-energy-group method in order to more accurately estimate the neutron population. It is especially important to determine this figure for a water-moderated reactor in which neutrons are emitted at fast energies and "disappear" at thermal energies. How does this phenomenon modify $k_{\infty}$ ? If we separate the neutron population into two separate groups, the fast and thermal energy groups, it must be remembered that the previous representation intuitively defines the ratio of the number of thermal neutrons to a generation divided by the number of thermal neutrons at the subsequent generation, since the "input" in Fig. 11.10 (left) is a neutron at thermal energy and the scheme ends with the absorption of a neutron at thermal energy. Inside a reactor, the phenomenon is obviously infinitely more complex than this schematic version. Using two energy groups leads to a further complexity with a cut-off energy that is situated between
the thermal energy $E_{t h}$ and the fast fission energy $E_{0}$. In 1960, E.C. Critoph ${ }^{5}$ formalized the equation for $k_{\infty}$ in (Heavy Water Lattices, p. 49) by supposing that the cut-off for the two groups is situated below the resonant absorption of ${ }_{92}^{238} U$ at energy $E_{c}$ in the following manner:

$$
k_{\infty 1}=\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right) \frac{1-r}{1-\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r}
$$

by introducing new definitions with respect to the four-factor formula. The quantity $r$ is the fraction of neutrons slowed down below the epithermal zone (having thus survived a resonant absorption), and having been absorbed by producing $r \eta\left(E_{c}\right) f$ $\left(E_{c}\right)$ new neutrons. $\eta\left(E_{c}\right)$ is the number of neutrons produced per neutron having survived the resonant absorption zone. This number differs from $\eta\left(E_{t h}\right)$, which is usually employed since in practice, $\eta$ depends on the incident neutron energy through the mean number of neutrons generated, as well as the energy dependence of cross sections. $f\left(E_{c}\right)$ is the utilization factor of epithermal neutrons that have survived the resonant absorption up to energy $E_{c}$. It differs from the usual $f\left(E_{t h}\right)$ for the same reason as does $\eta\left(E_{t h}\right)$. The demonstration of the previous formula is based on the definition of $k_{\infty}$ that leads to considering a cut-off point in the neutron production cycle, situated in Fig. 11.11 at the point represented by scissors. The definition of $k_{\infty}$ is then given as:

$$
k_{\infty 1}=\frac{\text { Number of thermal neutrons at generation } n+1}{\text { Number of thermal neutrons at generation } n}
$$

Thermal neutrons created by a thermal neutron entering the sketch (from the left on Fig. 11.11) are counted by determining all thermal neutrons produced by the entering neutron and preventing any neutrons from reaching the cut-off value (Fig. 11.12).

$$
\begin{aligned}
k_{\infty 1} & =\frac{\overbrace{\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right)(1-r)}^{\text {first cut-off }}+\overbrace{\eta\left(E_{t h}\right) \eta\left(E_{c}\right) f\left(E_{c}\right) r \varepsilon^{2} p^{2}(1-r) f\left(E_{t h}\right)}^{\text {second cut-off }}+\overbrace{\eta\left(E_{t h}\right) \eta\left(E_{c}\right)^{2} f\left(E_{c}\right)^{2} r^{2} \varepsilon^{3} p^{3}(1-r) f\left(E_{t h}\right)}^{\text {third cut-off }}+. .}{1} \\
& =\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right)(1-r)\left[1+\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r+\left(\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r\right)^{2}+\left(\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r\right)^{3}+\ldots\right]
\end{aligned}
$$

Since $r$ is small, the term $\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r$ is less than 1.

[^254]

Fig. 11.11 Two-group $k_{\infty}$ theory


Fig. 11.12 Neutron count at thermal cut-off

$$
\begin{aligned}
k_{\infty 1}=\lim _{n \rightarrow+\infty}\left(\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right)(1-r)\right. & \left.\frac{1-\left(\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r\right)^{n}}{\left[1-\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r\right]}\right) \\
& =\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right)(1-r) \frac{1}{\left[1-\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r\right]}
\end{aligned}
$$

This calculation counts all the thermal neutrons generated by the "upper" route for all the successive generations on the previous sketch. The thermal cut-off level is relatively arbitrary and it could in fact have been placed at the epithermal level in similar fashion to produce a new and equally valid definition of $k_{\infty}$ :
$k_{\infty 2}=\frac{\text { Number of neutrons produced by epithermal absorption atgenerationn }+1}{\text { Number of neutrons produced by epithermal absorption atgenerationn }}$

$$
k_{\infty 2}=\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p \frac{r}{1-\eta\left(E_{t h}\right) f\left(E_{t h}\right) \varepsilon p(1-r)}
$$

In this case, we must be careful that the input neutron in Fig. 11.13 (on the left) is one produced after an epithermal absorption and that factor $\eta$ does not appear at the beginning of the cycle (counting the latter would be equivalent to counting neutrons from the previous generation). Thus:

$$
\begin{aligned}
k_{\infty 2}= & \overbrace{\eta\left(E_{c}\right) f\left(E_{c}\right) r \varepsilon p}^{\text {first cut-off }}+\overbrace{\eta\left(E_{c}\right) f\left(E_{c}\right) r \varepsilon p(1-r) \eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right)}^{\text {second cut-off }}+\overbrace{\ldots . .}^{\text {third term }} \\
k_{\infty 2} & =\lim _{n \rightarrow \infty}\left(\eta\left(E_{c}\right) f\left(E_{c}\right) r \varepsilon p \frac{1-\left(\varepsilon p \eta\left(E_{t h}\right) f\left(E_{t h}\right)(1-r)\right)^{n}}{\left[1-\varepsilon p \eta\left(E_{t h}\right) f\left(E_{t h}\right)(1-r)\right]}\right) \\
& =\eta\left(E_{c}\right) f\left(E_{c}\right) r \varepsilon p \frac{1}{\left[1-\varepsilon p \eta\left(E_{t h}\right) f\left(E_{t h}\right)(1-r)\right]}
\end{aligned}
$$

It can be seen that the expression for the infinite multiplication coefficient differs according to the definition of the cut-off used. This result is particularly counterintuitive compared to the idea that any given state of a reactor corresponds to a specific reactivity. The problem arises since the four-factor formula is a calculation based on specific fission neutrons (either neutrons produced after thermal absorption in the first case $\left[k_{\infty 1}\right]$, or else neutrons produced after epithermal absorption in the second case, $\left.\left[k_{\infty 2}\right]\right)$. The method consists in measuring the increase in a given neutron population by comparing the number of particles of a given age between two successive generations. The result consequently differs according to the actual


Fig. 11.13 Neutron count at epithermal cut-off
age in question. If $k_{\infty}$ were calculated on the basis of a number of reaction rates, this number would concern neutrons produced through all types of fission irrespective of their origin, thus giving a single definition. To use a demographics analogy, this approach would be the equivalent of calculating an increase in the neutron population by counting the number of births and deaths. However, stability of the reactor at criticality (i.e. stability of the population in the demographics analogy) is indeed the reality that must be reflected by the two definitions of $k_{\infty}$. Hence, it may be seen that while the two values of $k_{\infty}$ obtained using the two cut-off values are very different, the criticality condition in infinite medium is the same for both approaches, and that:

$$
\left\{\begin{array}{c}
k_{\infty 1}=\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right) \frac{1-r}{1-\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r}=1 \\
k_{\infty 2}=\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p \frac{r}{1-\eta\left(E_{t h}\right) f\left(E_{t h}\right) \varepsilon p(1-r)}=1
\end{array}\right.
$$

corresponds to the same equation as:

$$
\eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right)(1-r)=1-\eta\left(E_{c}\right) f\left(E_{c}\right) \varepsilon p r
$$

Reasoning is the same regardless of the cut-off value used to count neutrons. The criticality condition expresses the same neutron balance for any counting method. Let us now consider a finite reactor. The leakage probabilities should be employed outside the reactor geometry. $P\left(E_{0} \rightarrow E_{c}\right)=1 /\left(1+L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right) B^{2}\right)$ is the non-leakage probability for a neutron as it slows down to the cut-off of the thermal group, while $P\left(E_{c} \rightarrow E_{t h}\right)=1 /\left(1+L_{s}^{2}\left(E_{c} \rightarrow E_{t h}\right) B^{2}\right)$ is the non-leakage probability of a neutron during slowing down in the thermal group. Note that the product:

$$
P\left(E_{0} \rightarrow E_{c}\right) P\left(E_{c} \rightarrow E_{t h}\right)=P\left(E_{0} \rightarrow E_{t h}\right)=\frac{1}{\left(1+L_{s}^{2}\left(E_{0} \rightarrow E_{t h}\right) B^{2}\right)}
$$

is the non-leakage probability of the neutron throughout its slowing down, $L_{s}$ being the slowing-down length. It should also be noted that this equation relates $L_{s}^{2}\left(E_{0} \rightarrow E_{\text {th }}\right)$ to $L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right)$ and $L_{s}^{2}\left(E_{c} \rightarrow E_{t h}\right) . P_{E_{t h}}=1 /\left(1+L^{2} B^{2}\right)$ is also defined as the non-leakage probability of the neutron at thermal energy, with $L$ being the thermal scattering length. In the case of the cut-off cycle illustrated in Fig. 11.14 by the scissors, the following is obtained:


Fig. 11.14 Neutron cut-off cycle located at the scissors in a two-energy-group calculation with geometrical leakage

$$
\begin{aligned}
k_{e f f 1} & =\eta\left(E_{t h}\right) \varepsilon p \underbrace{P\left(E_{0} \rightarrow E_{c}\right) P\left(E_{c} \rightarrow E_{t h}\right)}_{P\left(E_{0}-E_{t h}\right)} P_{t h} f\left(E_{t h}\right) \frac{1-r}{1-\eta\left(E_{c}\right) f\left(E_{c}\right) P\left(E_{0} \rightarrow E_{c}\right) \varepsilon p r} \\
& =\eta\left(E_{t h}\right) \varepsilon p \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{t h}\right) B^{2} 1+L^{2} B^{2}} f\left(E_{t h}\right) \frac{1-r}{1-\eta\left(E_{c}\right) f\left(E_{c}\right) \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right) B^{2}} \varepsilon p r}
\end{aligned}
$$

Similarly, another cut-off situated on the epithermal track gives a different evaluation of $k_{\text {eff }}$, i.e. $k_{\text {eff } 2}$ :

$$
\begin{aligned}
k_{e f f 2} & =\eta\left(E_{c}\right) f\left(E_{c}\right) P\left(E_{0} \rightarrow E_{c}\right) \varepsilon p \frac{r}{1-\eta\left(E_{t h}\right) \varepsilon p \underbrace{P\left(E_{0} \rightarrow E_{c}\right) P\left(E_{c} \rightarrow E_{t h}\right)}_{P\left(E_{0}-E_{t h}\right)} P_{t h}(1-r) f\left(E_{t h}\right)} \\
& =\eta\left(E_{c}\right) f\left(E_{c}\right) \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right) B^{2}} \varepsilon p \frac{r}{1-\eta\left(E_{t h}\right) \varepsilon p \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{t h}\right) B^{2} 1+L^{2} B^{2}}(1-r) f\left(E_{t h}\right)}
\end{aligned}
$$

As with $k_{\infty}$, it may be seen that the two definitions of $k_{\text {eff }}$ are different but that the criticality condition is identical in both cases:

$$
\begin{gathered}
k_{\text {eff } 1}=1 \Rightarrow \eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right) \frac{1-r}{1-\eta\left(E_{0}\right) f\left(E_{0}\right) \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right) B^{2}} \varepsilon p r} \\
=\left(1+L_{s}^{2}\left(E_{0} \rightarrow E_{t h}\right) B^{2}\right)\left(1+L^{2} B^{2}\right) \\
k_{e f f 2}=1 \Rightarrow \\
\Rightarrow \quad \eta\left(E_{c}\right) f\left(E_{c}\right) \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right) B^{2}} \varepsilon p r \\
\\
=1-\eta\left(E_{t h}\right) \varepsilon p \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{t h}\right) B^{2}} \frac{1}{1+L^{2} B^{2}}(1-r) f\left(E_{t h}\right) \\
\Rightarrow \quad \eta\left(E_{t h}\right) \varepsilon p f\left(E_{t h}\right) \times \frac{1-r}{1-\eta\left(E_{c}\right) f\left(E_{c}\right) \frac{1}{1+L_{s}^{2}\left(E_{0} \rightarrow E_{c}\right) B^{2}} \varepsilon p r} \\
\quad=\left(1+L_{s}^{2}\left(E_{0} \rightarrow E_{t h}\right) B^{2}\right)\left(1+L^{2} B^{2}\right)
\end{gathered}
$$

Although it is more complicated, the previous formulae may be generalized out in a multi-group formalism and using indices for the various probabilities and the branching ratio by the group number being considered. For example, calculation of $k_{\infty}$ for 3 energy groups (one fast group noted 1, two thermal groups denoted by 2 and 3 and the thermal state corresponding to index 4) gives:

$$
\left\{\begin{array}{l}
k_{\infty 1}=\eta \varepsilon \operatorname{p} f\left(\frac{1-r_{1}}{1-\varepsilon p \eta_{1} f_{1} r_{1}}\right)\left(\frac{1-r_{2}}{1-\frac{p \eta_{2} f_{2} r_{2}\left(1-r_{1}\right)}{1-\varepsilon p \eta_{1} f_{1} r_{1}}}\right) \\
k_{e f f 1}=\eta \varepsilon p f P_{1} P_{2} P_{3} P_{4}\left(\frac{1-r_{1}}{1-\varepsilon p P_{1} \eta_{1} f_{1} r_{1}}\right)\left(\frac{1-r_{2}}{1-\frac{p P_{1} P_{2} \eta_{2} f_{2} r_{2}\left(1-r_{1}\right)}{1-\varepsilon p P_{1} \eta_{1} f_{1} r_{1}}}\right)
\end{array}\right.
$$

### 11.5 Multiplication Factor Through a Reaction Rate Balance

The ambiguous definition of the consecutive terms of the four factors has been removed in calculation codes that discretize the energy spectrum of neutrons in bands/groups and compute the group-wise reaction rate. In particular, the strong hypothesis of the four-factor formula consists in localizing the resonant absorption after having applied factor $\varepsilon$. It becomes more ambiguous in a multi-group approach where fast fission is possible in several fast groups and where resonances are located in several epithermal groups. Thus, the difference between the application of $\varepsilon$ and $p$ makes the use of the four-factor formula obsolete. The effective
multiplication factor represents the mean number of neutrons emitted by fission per neutron emitted by fission in the reactor. It is given by the neutron balance as follows:

$$
\begin{equation*}
\text { Definition of } k_{\text {eff }}=\frac{\text { number of neutrons emitted by fission }}{\text { number of neutrons lost in reactor }} \tag{11.4}
\end{equation*}
$$

Hence, the rate at which neutrons disappear from the reactor is introduced in that equation. It accounts for:

- neutron absorptions (fission and capture),
- absorption by excess reactions (by reaction ( $n, 2 n$ ), ( $n, 3 n$ ), etc.) that are not usually counted in absorptions,
- the leakages from the reactor.

It should be noted that excess reactions are not influenced by $k_{\text {eff }}$ since a neutron absorbed by $(n, 2 n)$ produces two neutrons for any multiplying medium that is considered. Indeed, this is also the case for $(n, x n)$ reactions. The balance is written as follows:

Leakages + Absorptions + Absorptions by excess reactions

$$
=\frac{\text { Productions }}{k_{e f f}}+\text { Excess Productions }
$$

Absorptions by excess reactions

$$
=\int_{\text {Energy }} \int_{\text {reactor }}\left(\Sigma_{n, 2 n} \Phi+\Sigma_{n, 3 n} \Phi+\Sigma_{n, 4 n} \Phi+\ldots\right) d^{3} r d E
$$

ExcessProductions $=\int_{\text {Energy reactor }} \int_{n, 2 n}\left(2 \Sigma_{n} \Phi+3 \Sigma_{n, 3 n} \Phi+4 \Sigma_{n, 4 n} \Phi+\ldots\right) d^{3} r d E$
$k_{\text {eff }}=\frac{\int_{\text {Energy reactor }} \int_{\text {Energy }} \int_{f} \Phi d^{3} r d E}{\int_{\text {reactor }}\left(\Sigma_{a} \Phi-\Sigma_{n, 2 n} \Phi-2 \Sigma_{n, 3 n} \Phi-3 \Sigma_{n, 4 n} \Phi+\ldots\right) d^{3} r d E+\text { Leakages }}$
The previous formulation supposes that the absorption cross section does not account for the excess production cross sections by reactions ( $n, 2 n$ ), ( $n, 3 n$ ), etc. Usually, in diffusion theory with the fundamental mode, neutron leakage from the reactor (which will be discussed later on) is expressed as:

$$
\text { Leakages }=\int_{\text {Energy reactor }} \int_{\text {Energy reactor }}-D \Delta \Phi d^{3} r d E=\int_{g} D B_{g}^{2} \Phi d^{3} r d E
$$

Inserting the migration area in one-group theory:

$$
M^{2} \equiv \frac{\int D \Phi d E}{\int \Sigma_{a} \Phi d E}
$$

and the definition of the infinite multiplication factor:

$$
k_{\infty} \equiv \frac{\int_{\text {Energy }} \int_{\text {reactor }} v \Sigma_{f} \Phi d v d E}{\int_{\text {Energy reactor }} \int_{a} \Phi d v d E}
$$

leads to the formula that relates $k_{\text {eff }}$ and $k_{\infty}$, without accounting for the excess productions:

$$
k_{e f f}=\frac{k_{\infty}}{\left(1+M^{2} B_{g}^{2}\right)}
$$

It should be noted that the definition of $k_{\infty}$ implies that the latter depends on the spectrum of the reactor in question, and thus in particular on leakage therein. In practice, the calculation of a critical configuration is carried out with buckling corresponding to the fundamental mode.

Furthermore, it is possible to expand the expression of $k_{\text {eff }}$ as a balance of reaction rates (Fig. 11.15 for a $U O X$ core and Fig. 11.16 for a MOX core, both fuel types being equivalent in terms of cycle lengths ${ }^{6}$ ), specifying that:

- neutrons are produced from fissile nuclides:
- regardless of incident neutron energy (such as ${ }_{92}^{235} U$, denoted as $P_{5}$ for simplification),
- that are fissile only in fast spectrum (like ${ }_{92}^{238} U$, denoted $P_{8}$ for the sake of clarity),
- the absorption rate may be broken down into:
- resonant absorption on fertile nuclides (principally by ${ }_{92}^{238} U$, noted as $A_{\text {reson }}$ ),
- non-resonant absorption on fissile nuclides (effect of cross sections varying in $1 / v$, noted as $A_{t h}$ ),
- absorption on non-fissile structures (grids, boron, etc., noted as $A_{\text {structures }}$ ),

[^255]

| ${ }_{92}^{234} U$ Fertile captures | $\mathbf{1 0 4}$ |
| :--- | ---: |
| ${ }_{92}^{238} U$ Fertile captures | $\mathbf{2 4} \mathbf{2 9 3}$ |
| ${ }_{92}^{238} \mathrm{Pu}$ Fertile captures | $\mathbf{5 9}$ |
| ${ }_{94}^{240} \mathrm{Pu}$ Fertile captures | $\mathbf{5 4 1 5}$ |
| Total | $\mathbf{2 9 8 7 1}$ |


| Moderator captures | $\mathbf{3 2 2 5}$ |
| :--- | ---: |
| Boron captures | $\mathbf{2 9 7 8}$ |
| Sterile captures on | $\mathbf{1 2 2 3}$ |
| structures |  |
| Oxygen captures | $\mathbf{1 6 0}$ |
| Xenon 135 | $\mathbf{1 9 3 1}$ |
| Other FPs | $\mathbf{7 0 5 5}$ |
| Heavy nuclides | $\mathbf{1 4 3 7 1}$ |
| Total |  |

$$
\begin{aligned}
& k_{\text {eff }}=\frac{P_{5}+P_{8}}{A_{\text {total }}+\text { Leakages }} \\
& =\frac{100000}{37591+29871+30943+1595}=1.00000
\end{aligned}
$$

Fig. 11.15 Neutron balance for a homogeneous core with a quarter fractional core management for $U O X$ fuel with $3.7 \%$ enrichment in ${ }_{92}^{235} U$ at equilibrium at EOC, with a mean burn-up of $26,250 \mathrm{MWd} /$ ton (simulation of mean depletion with 500 ppm of boron)


| Moderator captures | $\mathbf{1 2 8 2}$ |
| :--- | ---: |
| Boron captures | $\mathbf{1 1 0 0}$ |
| Sterile captures on | $\mathbf{9 3 6}$ |
| structures |  |
| Oxygen captures | $\mathbf{1 6 5}$ |
| Xenon 135 | $\mathbf{9 5 0}$ |
| Other FPs | $\mathbf{5 5 2 0}$ |
| Heavy nuclides | $\mathbf{1 9 6 5 4}$ |
| Total | $\mathbf{2 9 8 0 7}$ |



Fig. 11.16 Neutron balance for a homogeneous core with a quarter fractional core management for $M O X$ fuel with $8.65 \%$ plutonium content at equilibrium at EOC, with a mean burn-up of $25,000 \mathrm{MWd} /$ ton (simulation of mean depletion with 500 ppm of boron)
to give the following equation:

$$
\begin{aligned}
k_{\infty} & =\frac{\text { Production }}{\text { Absorption }}=\frac{P_{5}+P_{8}}{A_{\text {reson }}+A_{\text {th }}+A_{\text {structures }}} \\
& =\frac{P_{5}+P_{8}}{P_{5}} \frac{P_{5}}{A_{\text {th }}} \frac{A_{\text {th }}}{A_{\text {reson }}+A_{\text {th }}} \frac{A_{\text {reson }}+A_{\text {th }}}{A_{\text {reson }}+A_{\text {th }}+A_{\text {structures }}}
\end{aligned}
$$

From this, a precise definition of the coefficients from the four-factor formula may be deduced:

$$
\varepsilon=\frac{P_{5}+P_{8}}{P_{5}}, \quad \eta=\frac{P_{5}}{A_{t h}}, \quad p=\frac{A_{\text {th }}}{A_{\text {reson }}+A_{t h}}, f=\frac{A_{\text {reson }}+A_{\text {th }}}{A_{\text {reson }}+A_{\text {th }}+A_{\text {structures }}}
$$

In the usual presentation of the four-factor formula, a chronological approach is employed. Indeed, the fast fission coefficient $\varepsilon$ is introduced as the fast fission generator. The previous calculation introduces a distinction between target nuclei that are basically those present in thermal reactors. In a fast reactor, all isotopes undergo fission in the fast spectrum and the specific case of ${ }_{92}^{238} U$ is without meaning. Similarly, in a water reactor, the use of plutonium in the MOX fuel requires the introduction of production terms by fission of fissile plutonium isotopes as well as resonant absorption on those isotopes. The thermal fissile isotopes are hence $\left({ }_{92}^{235} U,{ }_{94}^{239} P u,{ }_{94}^{241} P u\right)$, while the fertile ones, which after capture form an isotope in the thermal domain, are $\left({ }_{92}^{238} \mathrm{U},{ }_{94}^{238} \mathrm{Pu},{ }_{94}^{240} \mathrm{Pu},{ }_{94}^{242} \mathrm{Pu},{ }_{95}^{241} \mathrm{Am}\right)$.

$$
\varepsilon=\frac{P_{\text {fissile }}+P_{\text {fertile }}}{P_{\text {fissile }}}, \eta=\frac{P_{\text {fissile }}}{A_{\text {fissile }}}, p=\frac{A_{\text {fissile }}}{A_{\text {fertile }}+A_{\text {fissile }}}, f=\frac{A_{\text {fertile }}+A_{\text {fissile }}}{A_{\text {fertile }}+A_{\text {fissile }}+A_{\text {structure }}}
$$

The effect of burn-up is characterized by the appearance of fission products for which the sterile capture must be added to the absorption terms of structures. It can be seen that the neutrons originating from fast fissions are instantaneously recycled in the four-factor formula via the fast fission factor $\varepsilon$ (which is totaled using a multiplication factor applied to the number of neutrons produced by fission). These neutrons are not distinguished from the others in the calculation since the balance accounts for neutrons produced by any type of fission, regardless of the form of the incident neutron energy. The first approach is quite didactic and offers a natural means for understanding the kinetic aspects. However, it hinges on an arbitrary definition of fast and thermal neutrons, which is particularly well suited to thermal reactors, for which it has been developed.

### 11.6 Reactivity Effects or Reactivity Difference

Analysis of how a reactor responds to any variation of a physical parameter (temperature, composition, etc.) is often summarized in differential neutron coefficients. Whilst the mathematical definition of these coefficients is very precise
( $\partial k_{\text {eff }} / \partial T_{\text {comb }}$ is the fuel Doppler effect for example), their numerical evaluation may be quite difficult, especially for the composition of these effects: how can two distinct reactor states be precisely compared? It is very common to use the reactivity value $\rho=\left(k_{\text {eff }}-1\right) / k_{\text {eff }}$ having a critical value of 0 rather than the multiplication coefficient $k_{\text {eff }}$ determined in comparison to 1 . Under the nominal operating conditions of a reactor, $k_{\text {eff }}$ is very close to 1 and engineers have adopted the "bad" (but very practical for rapid calculation) habit of evaluating reactivity using the approximate formula $\rho \approx k_{\text {eff }}-1$. It can be seen that for wide variations in $k_{\text {eff }}$, this formula no longer gives consistent values as for the strict definition normalized by $k_{\text {eff. }}$ Hence, a reactivity difference between two states, $A$ and $B$, is given by the following formula:

$$
\text { Reactivity difference: } \quad \begin{align*}
\Delta \rho & =\rho_{B}-\rho_{A}=\frac{k_{e f f}^{B}-1}{k_{e f f}^{B}}-\frac{k_{e f f}^{A}-1}{k_{e f f}^{A}} \\
& =\frac{1}{k_{e f f}^{A}}-\frac{1}{k_{e f f}^{B}}=-\Delta\left(\frac{1}{k_{e f f}}\right) \tag{11.5}
\end{align*}
$$

However, the reactivity effect is defined as:

$$
\begin{equation*}
\text { Reactivity effect: } \quad \Delta \ln k_{e f f}=\ln k_{e f f}^{B}-\ln k_{e f f}^{A}=\ln \frac{k_{e f f}^{B}}{k_{e f f}^{A}} \tag{11.6}
\end{equation*}
$$

It may be seen that both definitions obey the additivity of the integral (the relation of Chasles), i.e. $\Delta \rho_{A C}=\Delta \rho_{A B}+\Delta \rho_{B C}$ and $\Delta \log _{\text {eff } A C}=\Delta \ln k_{\text {effAB }}+$ $\Delta \ln k_{\text {eff } B C}$. However, only the reactivity effect has the factorization property. If we consider a set of states $A_{i}$, corresponding to a multiplication coefficient $k_{\text {eff }}^{A_{i}}$, that is perturbed proportionally to obtain a multiplication factor of $\alpha k_{e f f}^{A_{i}}$, the reactivity effect will always be:

$$
\Delta \ln k_{e f f}=\ln \frac{\alpha k_{e f f}}{k_{\text {eff }}}=\ln \alpha
$$

and it is thus independent of the initial multiplication factor, which is not the case for the reactivity difference.

### 11.6.1 Comparison of the Effects on a UOX Fuel

We can illustrate the foregoing by calculating the fuel Doppler effect in infinite lattice ${ }^{7}$ for a $P W R$ uranium oxide pin enriched at $4.2 \%{ }_{92}^{235} U$ and for a mean

[^256]temperature variation of $540-286^{\circ} \mathrm{C}$ ("cold" Doppler effect). Physically, reactivity increases as fuel temperature decreases (stabilizing power of the Doppler effect in the case of a fuel temperature excursion). Here, the goal is to quantify the variation of the Doppler effect during the lifecycle of the fuel (e.g. between the Beginning Of Life, BOL, and End Of Life, EOL) in a reactor up to $50,000 \mathrm{MWd} /$ ton, Table 11.4).

These results show that while the reactivity effect increases slightly by 180 pcm during the cycle, the reactivity difference increases by 453 pcm . These figures both illustrate the same fact: the hardening of the neutron spectrum during burn-up, which may be observed by the increase in the spectrum index (ratio of the fast flux to the thermal flux with a cadmium cut-off at 0.625 eV ). Hence, there are preferential resonant capture reactions of ${ }_{92}^{238} U$ and the Doppler effect increases along the cycle.

However, the weight of this effect, which may be considered practically constant at around $877 \mathrm{pcm} \pm 90 \mathrm{pcm}$ using the "reactivity effect" approach, increases using the "reactivity difference" approach due to the significant decrease of $k_{\text {eff. }}$ Let us now consider the effect of boron concentration in the moderator and the impact of adding 500 ppm of boron to the previous fuel and calculate the reactivity effect and the difference in reactivity (Table 11.5). It may be seen that there is a hardening of the spectrum with burn-up, resulting in a decrease in the reactivity effect of boron, a powerful thermal absorbing material. At the same time, the reactivity difference due to boron increases since its relative contribution in a fuel with a low $k_{\text {eff }}$ value increases. In conclusion, the reactivity effect may be used to reduce the impact of the lowering of $k_{\text {eff }}$ with regard to the differential coefficient. Nonetheless, the reactivity difference will give the correct differential coefficient for a critical core where both definitions are the same, since for a small perturbation $\alpha$ (close to 1 ) near to the critical state ( $k_{\text {eff }}$ approaching 1 ):

$$
\left\{\begin{array}{l}
\Delta \ln k_{e f f}=\ln \frac{\alpha k_{e f f}}{k_{\text {eff }}}=\ln \alpha \approx \alpha-1 \\
\Delta \rho=\frac{\alpha k_{\text {eff }}-1}{\alpha k_{e f f}}-\frac{k_{e f f}-1}{k_{\text {eff }}}=\frac{\alpha-1}{\alpha k_{e f f}} \approx \alpha-1
\end{array}\right.
$$

An increase in the spectrum index (hardening) of a fuel, followed by a decrease (thermalization), would lead to a decrease in the boron reactivity effect followed by an increase almost concomitantly.

### 11.6.2 Reactivity Effect of Isotopic Change

From the global reactivity effect:

$$
\Delta \rho=\rho_{B}-\rho_{A}=\frac{1}{k_{e f f}^{A}}-\frac{1}{k_{e f f}^{B}}=\frac{k_{e f f}^{B}-k_{e f f}^{A}}{k_{e f f}^{A} k_{e f f}^{B}}
$$

Table 11.4 Cold Doppler effect ( -254 K ) and reactivity effect for UOX 4.2\% fuel

| Burnup $_{[\mathrm{MWd} / \text { /on] }}$ | 0 | 4000 | 8000 | 12,000 | 18,000 | 24,000 | 36,000 | 48,000 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $k_{\text {eff }}^{540{ }^{\circ} \mathrm{C}}$ | 1.28690 | 1.23298 | 1.18580 | 1.14611 | 1.09469 | 1.04912 | 0.97112 | 0.90585 |
| $k_{\text {eff }}^{286{ }^{\circ} \mathrm{C}}$ | 1.29706 | 1.24266 | 1.19537 | 1.15592 | 1.10469 | 1.05903 | 0.98054 | 0.91466 |
| $\Phi_{1} / \Phi_{2[-]}$ | 7.61 | 8.34 | 8.88 | 9.27 | 9.67 | 9.91 | 10.13 | 10.19 |
| $\Delta \ln k_{\text {eff }}$ [pcm] | 787 | 782 | 803 | 852 | 909 | 941 | 966 | 967 |
| $\Delta \rho_{\text {[pcm] }}$ | 609 | 632 | 645 | 740 | 827 | 892 | 989 | 1062 |

Table 11.5 Boron effect (+500 ppm) and reactivity effect for UOX $4.2 \%$ fuel

| Burnup $_{[\text {MWd/ton }]}$ | 0 | 4000 | 8000 | 12,000 | 18,000 | 24,000 | 36,000 | 48,000 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $k_{\text {eff }}^{500 \mathrm{ppm}}$ | 1.28690 | 1.23298 | 1.18580 | 1.14611 | 1.09469 | 1.04912 | 0.97112 |  |
| $k_{\text {eff }}^{0} \mathrm{ppm}$ | 1.33210 | 1.27338 | 1.22324 | 1.18152 | 1.12794 | 1.08082 | 1.00068 |  |
| $\Phi_{1} / \Phi_{2[-]}$ | 7.61 | 8.34 | 8.88 | 9.27 | 9.67 | 9.91 | 10.13 | 0.93383 |
| $\Delta \ln k_{\text {eff }[\mathrm{pcm}]}$ | 3452 | 3225 | 3108 | 3043 | 2992 | 2977 | 2998 |  |
| $\Delta \rho_{[\mathrm{pcm}]}$ | 2637 | 2573 | 2581 | 2615 | 2692 | 2796 | 3042 |  |

The reactivity effect induced by change in the concentration of a single isotope is obtained as follows:

$$
\Delta \rho=\frac{k_{e f f}^{B}-k_{e f f}^{A}}{k_{e f f}^{A} k_{e f f}^{B}}=\frac{\frac{v \Sigma_{f}^{B}}{\Sigma_{a}^{B}}-k_{e f f}^{A}}{k_{e f f}^{A} \frac{v \Sigma_{f}^{B}}{\Sigma_{a}^{B}}}=\frac{\frac{v \Sigma_{f}^{B}}{k_{e f f}^{A}}-\Sigma_{a}^{B}}{v \Sigma_{f}^{B}}=\frac{\frac{v \Sigma_{f}^{A}}{k_{e f f}^{A}}+\frac{\Delta\left(v \Sigma_{f}\right)}{k_{e f f}^{A}}-\left(\Sigma_{a}^{A}+\Delta\left(\Sigma_{a}\right)\right)}{v \Sigma_{f}^{B}}
$$

Since $\frac{v \Sigma_{f}^{A}}{k_{e f f}^{A}}-\Sigma_{a}^{A} \equiv 0$, the following equation is obtained:

$$
\Delta \rho=\frac{\frac{\Delta\left(v \Sigma_{f}\right)}{k_{e f f}^{A}}-\Delta\left(\Sigma_{a}\right)}{v \Sigma_{f}^{B}}
$$

The contribution of an isotope $i$ is given by:

$$
\begin{aligned}
\Delta \rho_{i} & =\frac{\frac{\Delta\left(\nu N_{i} \sigma_{f}^{i}\right)}{k_{e f f}^{A}}-\Delta\left(N_{i} \sigma_{a}^{i}\right)}{\nu \Sigma_{f}^{B}} \\
& =\frac{\left(\frac{\nu \sigma_{f}^{i}}{k_{e f f}^{A}}-\sigma_{a}^{i}\right) \Delta N_{i}}{\nu \Sigma_{f}^{B}}+\frac{N_{i}\left(\frac{\Delta\left(\nu \sigma_{f}^{i}\right)}{k_{e f f}^{A}}-\Delta \sigma_{a}^{i}\right)}{v \Sigma_{f}^{B}}+\frac{\Delta N_{i}\left(\frac{\Delta\left(\nu \sigma_{f}^{i}\right)}{k_{e f f}^{A}}-\Delta \sigma_{a}^{i}\right)}{\nu \Sigma_{f}^{B}}
\end{aligned}
$$

Three terms appear: the first is directly proportional to the difference in concentration $\Delta N_{i}$, the second is a spectral effect, i.e. a change induced by the impact of spectrum shift on the cross sections, and the third is a second-order effect.

### 11.7 Calculation of Reactivity by Perturbation Theory Estimate

(Marchuk 1959, p. 148; Planchard 1995, p. 315)
Let us consider the time-dependent Boltzmann equation without any independent sources (i.e. only fission sources), written using the transport operator $H$ :

$$
H[\Phi]=\frac{1}{v} \frac{\partial \Phi}{\partial t}
$$

A stationary solution exists if and only if $H\left[\Phi_{0}\right]=0$, thus if the transport operator $H$ has a zero eigenvalue. Mathematically, a parameter $\lambda$ is defined such that for a given critical value $\lambda_{0}$, the operator $H\left(\lambda_{0}\right)$ has a zero eigenvalue. The reactor defined
by $H\left(\lambda_{0}\right)$ is thus the associated critical reactor for the true reactor defined by the operator $H$. The critical flux $\Phi_{0}$ and the adjoint critical flux $\Phi_{0}^{*}$ are defined as:

$$
H\left(\lambda_{0}\right)\left[\Phi_{0}\right]=H_{0}\left[\Phi_{0}\right]=0 \quad \text { and } \quad H^{*}\left(\lambda_{0}\right)\left[\Phi_{0}^{*}\right]=0
$$

Let us now consider a reactor subject to any form of mild perturbation (slight rod insertion, small temperature increase, etc.). This reactor would be critical for a flux solution that is also perturbed, and the perturbation $\delta \Phi_{0}$ satisfies the same boundary conditions as $\Phi_{0}$ :

$$
\begin{aligned}
\left(H_{0}+\delta H_{0}\right)\left[\Phi_{0}+\delta \Phi_{0}\right]= & 0 \quad \text { or even : } \\
& \underbrace{H_{0}\left[\Phi_{0}\right]}_{0}+\delta H_{0}\left[\Phi_{0}\right]+H_{0}\left[\delta \Phi_{0}\right]+\delta H_{0}\left[\delta \Phi_{0}\right]=0
\end{aligned}
$$

This equation has an infinite number of solutions in $\delta \Phi_{0}$ since if $\delta \Phi_{0}$ is a solution so too is $\delta \Phi_{0}{ }^{\prime}=\delta \Phi_{0}+\alpha\left(\Phi_{0}+\delta \Phi_{0}\right)$ for any value of the constant term $\alpha$. Thus, $\delta \Phi_{0}$ can be calculated with a chosen normalization condition that does not modify the reactivity value. However, to obtain the value of the flux perturbed by measuring a local signal (e.g. in a local fuel substitution experiment), the normalization condition must be consistent with the experiment, for instance, a constant flux at a position in a fission chamber far removed from the perturbed region. ${ }^{8}$

By applying the operator:
$<\Phi_{0}^{*}, f(r, E)>=\int_{\text {reactor }} d^{3} r \int_{0}^{\infty} \Phi_{0}^{*}(r, E) f(r, E) \Phi(r, E) d E$, the following equation is obtained:

$$
<\Phi_{0}^{*}, \delta H_{0}\left[\Phi_{0}\right]>+<\Phi_{0}^{*}, H_{0}\left[\delta \Phi_{0}\right]>+<\Phi_{0}^{*}, \delta H_{0}\left[\Delta \Phi_{0}\right]>=0
$$

Since $<\Phi_{0}^{*}, H_{0}\left[\delta \Phi_{0}\right]>=<H_{0}^{*}\left[\Phi_{0}^{*}\right], \delta \Phi_{0}>=<0, \delta \Phi_{0}>=0$ as $H_{0}^{*}\left[\Phi_{0}^{*}\right]=0$ by definition, the equation may be simplified to:

$$
<\Phi_{0}^{*}, \delta H_{0}\left[\Phi_{0}\right]>+<\Phi_{0}^{*}, \delta H_{0}\left[\delta \Phi_{0}\right]>=0
$$

At this point, the perturbation equation is accurate but it requires that the solution to the critical perturbed reactor be found (to obtain $\delta \Phi_{0}$ ), which is not of any great practical use. For small perturbations, the second term can be neglected: $<\Phi_{0}^{*}, \delta H_{0}\left[\delta \Phi_{0}\right]>\approx 0$. Hence: $<\Phi_{0}^{*}, \delta H_{0}\left[\Phi_{0}\right]>=0$. Introducing the neutron production operator $P$ and the loss operator $K$, the transport operator may be written as:

[^257]$$
H_{0}[]=\lambda_{0} P[]-K[]=\frac{P[]}{k_{e f f}}-K[]
$$

The perturbed operator is written as:

$$
H_{0}^{\prime}[]=\lambda_{0}^{\prime} P^{\prime}[]-K^{\prime}[]=\left(\lambda_{0}+\delta \lambda_{0}\right)(P[]+\delta P[])-(K[]+\delta K[])
$$

Thus: $\delta H[]=H_{0}^{\prime}[]-H_{0}[]=\left(\lambda_{0}+\delta \lambda_{0}\right)(P[]+\delta P[])-(K[]+\delta K[])-\lambda_{0} P[]+K[]$

$$
\approx \delta \lambda_{0} P[]+\lambda_{0} \delta P[]-\delta K[]
$$

which leads to : $\quad \Delta \lambda_{0}=\frac{<\Phi_{0}^{*},\left(\lambda_{0} \delta P-\delta K\right)\left[\Phi_{0}\right]>}{<\Phi_{0}^{*}, P\left[\Phi_{0}\right]>}$
or again, based on the fact that $\rho=\left(k_{\text {eff }}-1\right) / k_{\text {eff }}$ :

$$
\delta \rho=\frac{<\Phi_{0}^{*}, \delta H\left[\Phi_{0}\right]>}{<\Phi_{0}^{*}, P\left[\Phi_{0}\right]>} \quad \text { with } \quad \delta H[]=\frac{\delta P[]}{k_{e f}}-\delta K[]
$$

This formula is of great practical interest since only one critical flux and adjoint flux calculation under the reference conditions is required to obtain the perturbation in reactivity induced by a change in the transport operator, whether due to the material composition or to a change in the cross sections. From the 1970s to the 1990s, the perturbation method was used to compensate for the weak calculation power of computers, but during the 2000s, it has tended to be replaced by direct calculations without approximation of the order of the perturbation.

### 11.8 Evolution of the Reactivity Along the Cycle

To be able to exploit a reactor during a sufficient time, it is necessary to introduce some exceed of reactivity which must be compensated with the boron in the beginning of cycle. The Fig. 11.17 shows the evolution of the reactivity balance for a UOX $3.25 \%$ fuel. We shall note the weight of the saturated xenon is about 2800 pcm , that the weight of the moderating effect makes more than double during the cycle (from 2100 to 5400 pcm ), and that the boron ( $11,800 \mathrm{pcm}$, approximately 1300 ppm of boron) is adjusted in order to assure criticality. The loss of reactivity


Fig. 11.17 Reactivity effects versus time/burn up (3.25\% U235 fuel, cycle natural length $11,000 \mathrm{MWd} / \mathrm{t}$ )
during the cycle is due to the global disappearance of the fissile nuclei (because of fission) and to the concomitant appearance of absorbent fission products. The R rod bank, which is slightly inserted at the top of the core in the middle of its operating band, weighs approximately 200 pcm .

# Chapter 12 <br> Critical Homogeneous Reactor Theory 

The theoretical analysis of nuclear reactors began during World War II. The first steps in the race to acquire this knowledge took place in the United States with the construction of the Chicago Pile 1 (CP1) under the stands of the Chicago stadium. The simplest analysis consists in supposing that the pile is a homogeneous multiplying material for neutrons and the neutron flux is sought for under the criticality hypothesis. Mathematical calculations that are quite simple allow the study of the spatial flux distribution in a one-energy group theory.
(Meghreblian and Holmes 1960, p. 160).

### 12.1 Introduction

The word "pile" stems from the fact that the first critical reactor in Chicago was in fact a pile of graphite blocks which were used as a neutron-moderating material. On the right in Picture 12.1, we see a graphite block from the Fermi pile [CP1 for Chicago Physics One, also called West Stands Reactor (Stephenson 1954, p. 69)], one of the rare surviving pictures from that time. In Picture 12.1, we see the "flakes" of pure graphite bricks. The whole pile was made up of 57 layers of graphite ( 350 tons) and 6 tons of uranium metal, placed in a cubic lattice within the large graphite volume (De La Gorce 1992, p. 115; Pollard and Davidson 1956, p. 251), and of which only one picture remains (Barnaby 1971, p. 23). Since the amount of uranium metal available was not sufficient, 35 tons of uranium oxide were also used to finish the lattice. The global shape of the lattice was a sphere, minus its upper part, which was intended to become critical under a plastic cover to form a depression, thereby decreasing the amount of air absorbing neutrons. This set-up ultimately proved unusable, since the pile became critical even before it was completely assembled. It was subsequently dismantled before being rebuilt at Argonne.

If we consider a volume $V$ consisting of a homogeneous medium, and delimited by a surface area $S$, the Helmholtz equation, devised by Hermann Louis Ferdinand

Picture 12.1 A graphite block of the CP1 pile of Chicago (1941) (Public domain)


Von Helmholtz ${ }^{1}$ (1821-1894), is naturally used in situations involving neutron diffusion theory (Ferziger and Zweifel 1966, p. 31):

[^258]

[^259]\[

$$
\begin{equation*}
\text { Helmholtz equation: } \quad \Delta \Phi(\vec{r})+\lambda \Phi(\vec{r})=0 \tag{12.1}
\end{equation*}
$$

\]

The Helmholtz equation is a particular elliptic second-order partial differential equation, also known as the wave equation since it is formally similar to the wave equation in quantum physics (Bonilla 1957, p. 179: Etherington 1957, pp. 6-157). Several mathematical properties related to this eigenvalue problem can be obtained from (Planchard 1995; Wilkinson 1965), in its time-dependent form in (Crank 1975) and on the approximation of elliptic problems with boundary conditions in (Aubin 1972). In particular, the associated Green function that cancels out at infinity and provides a solution to the equation:

$$
\Delta G(\vec{r})+\lambda G(\vec{r})=-\delta(\vec{r})
$$

is written as $G(\vec{r})=e^{i \sqrt{\lambda} r} /(4 \pi r)$ in spherical geometry (Kanwal 1971, p. 116). For two-dimensional geometry, the solution is $G(\vec{r})=i H_{0}^{1}(\sqrt{\lambda}|r|) / 4$ where $H_{0}^{1}$ is the Hankel function. In general, if $\lambda$ is a complex number, the root $\sqrt{\lambda}$ is chosen such that its imaginary part is positive, so that $G(\vec{r})$ is zero at infinity. If $\lambda=\omega^{2}$ is a positive real number, the solution becomes $G(\vec{r})=e^{i \omega r} /(4 \pi r)$ in spherical coordinates $\left(G(\vec{r})=i H_{0}^{1}(\omega|r|) / 4\right.$ in $\left.2 D\right)$. If $\lambda=-\kappa^{2}$ is a negative real number, then $G(\vec{r})$ $=e^{-\kappa r} /(4 \pi r) \quad\left(G(\vec{r})=K_{0}(\kappa|r|) /(2 \pi)\right.$ in $2 D$ where $K_{0}$ is the modified Bessel function). ${ }^{2}$

To outline the problem of flux decomposition, we shall recall some mathematical properties that will be useful for the following parts. The Laplacian operator has associated eigenfunctions $\Phi_{k}$ such that:

$$
\Delta \Phi_{k}(\vec{r})+\lambda_{k} \Phi_{k}(\vec{r})=0
$$

The mathematical quantity $\lambda_{k}$ is called an eigenvalue, and several eigenfunctions may correspond to a given eigenvalue. The set of eigenfunctions forms a basis of functions, which forms a natural basis for expanding any function $\Phi(\vec{r})$ that verifies the Helmholtz equation if it is complete. If the space variable describes a finite volume, the set of eigenfunctions has a cardinality number-these can be indexed by a number, although it is infinite:

$$
\Phi(\vec{r})=\sum_{k} \phi_{k} \Phi_{k}(\vec{r})
$$

Several numerical methods may be employed to calculate the eigenvalues efficiently-some of these will be discussed in Chap. 18, amongst which the Rayleigh-Ritz variational method that gives the upper values and also the Weinstein variational method for lower values, which is a more complex problem (Gould 1966).

[^260]In reactor physics, we generally consider cases in which the flux satisfies the boundary conditions of $S$ surrounding a volume $V$. Either the flux is assumed to be zero at the boundary, or its derivative with respect to the normal is zero, i.e. a zero flux gradient corresponding to a flat flux at the interface (symmetry boundary conditions):

$$
\Phi(\vec{r} \in S)=0 \quad \text { or } \quad \frac{\partial \Phi}{\partial n}(\vec{r} \in S)=0
$$

The eigenfunctions that verify such a boundary condition form a complete basis having a maximum rank, i.e. no individual eigenfunction is a linear combination of the others. It can easily be shown that the eigenvalues of the Helmholtz equation with a given boundary condition are positive real numbers. Indeed, assuming that $\Phi_{k}(\vec{r})$ is a complex function (in the mathematical sense, i.e. $\Phi_{k}=\Phi_{R}+i \Phi_{i}$ where $i^{2}$ $=-1$ ), the Helmholtz equation can be multiplied by the conjugate function $\overline{\Phi_{k}}=\Phi_{R}-i \Phi_{i}$, and integrated over the considered volumes (space dependence is removed to simplify the notations):

$$
\int_{V} \overline{\Phi_{k}}\left(\Delta \Phi_{k}+\lambda_{k} \Phi_{k}\right) d \vec{r}=\int_{V} \overline{\Phi_{k}} \Delta \Phi_{k} d \vec{r}+\lambda_{k} \int_{V} \overline{\Phi_{k}} \Phi_{k} d \vec{r}=0
$$

and: $\int_{V} \overline{\Phi_{k}} \Phi_{k} d \vec{r}=\int_{V}\left|\Phi_{k}\right|^{2} d \vec{r} \geq 0$. The other integral is simplified using:

$$
\operatorname{div}\left(\overline{\Phi_{k}} \overrightarrow{\operatorname{grad}} \Phi_{k}\right)=\overline{\Phi_{k}} \Delta \Phi_{k}+\overrightarrow{\operatorname{grad}} \overline{\Phi_{k}} \cdot \overrightarrow{\operatorname{grad}} \Phi_{k}
$$

Hence, we have: $\int_{V} \overline{\Phi_{k}} \Delta \Phi_{k} d \vec{r}=\int_{V} \operatorname{div}\left(\overline{\Phi_{k}} \overrightarrow{\operatorname{grad}} \Phi_{k}\right) d \vec{r}-\int_{V} \overrightarrow{\operatorname{grad}} \overline{\Phi_{k}} \cdot \overrightarrow{\operatorname{grad}} \Phi_{k} d \vec{r}$
From the Ostrogradski theorem, the following is obtained: $\int_{V} \operatorname{div}\left(\overrightarrow{\Phi_{k}} \overrightarrow{\operatorname{grad}} \Phi_{k}\right) d \vec{r}=$ $\int_{S} \overline{\Phi_{k}} \overrightarrow{\operatorname{grad}} \Phi_{k} d S=0$ since either the flux is zero at the boundary, and its conjugate will also be zero, or its derivative is zero, and thus $\overrightarrow{\operatorname{grad}} \Phi_{k}=0$. Moreover:

$$
\begin{gathered}
\int_{V} \overrightarrow{\operatorname{grad}} \overline{\Phi_{k}} \cdot \overrightarrow{\operatorname{grad}} \Phi_{k} d \vec{r}=\int_{V}\left[\left(\frac{\partial \Phi_{R}}{\partial x}\right)^{2}+\left(\frac{\partial \Phi_{i}}{\partial x}\right)^{2}+\left(\frac{\partial \Phi_{R}}{\partial y}\right)^{2}+\left(\frac{\partial \Phi_{i}}{\partial y}\right)^{2}+\left(\frac{\partial \Phi_{R}}{\partial z}\right)^{2}+\left(\frac{\partial \Phi_{i}}{\partial z}\right)^{2}\right] d \vec{r} \geq 0 \\
\text { Hence }: \lambda_{k}=\frac{\int_{V} \overrightarrow{\operatorname{grad}} \overline{\Phi_{k}} \cdot \overrightarrow{\operatorname{grad}} \Phi_{k} d \vec{r}}{\int_{V} \overline{\Phi_{k}} \Phi_{k} d \vec{r}} \geq 0
\end{gathered}
$$

If $\Phi_{k}(\vec{r})$ verifies the Helmholtz equation and one of the boundary conditions given before, the eigenvalues are positive real numbers, or in other words, a Helmholtz equation with a negative coefficient $\lambda$ cannot have a solution that is zero on a finite domain. Moreover, if $\Phi_{k}$ is a solution, its conjugate $\overline{\Phi_{k}}$ is also a
solution. It can be proved that two different eigenfunctions of a bare reactor are orthogonal to each other in the sense of the volume integral (Planchard 1995, p. 58). Indeed, let $\Phi_{i}$ and $\Phi_{j}$ be two solutions such that:

$$
\left\{\begin{aligned}
\Delta \Phi_{i}+\lambda_{i} \Phi_{i} & =0 \\
\Delta \Phi_{j}+\lambda_{j} \Phi_{j} & =0
\end{aligned}\right.
$$

Multiplying the first equation by $\Phi_{j}$ and the second by $\Phi_{i}$, then subtracting one equation from the other (term-wise) after integration, the following equation is reached:

$$
\begin{gather*}
\int_{V} \Phi_{j} \Delta \Phi_{i} d \vec{r}-\int_{V} \Phi_{i} \Delta \Phi_{j} d \vec{r}+\left(\lambda_{i}-\lambda_{j}\right) \int_{V} \Phi_{j} \Phi_{i} d \vec{r}=0 \\
\int_{V} \Phi_{j} \Delta \Phi_{i} d \vec{r}-\int_{V} \Phi_{i} \Delta \Phi_{j} d \vec{r}=\underbrace{}_{\underbrace{}_{V}\left[\operatorname{div}\left(\Phi_{j} \overrightarrow{\operatorname{grad}} \Phi_{i}\right)-\operatorname{div}\left(\Phi_{i} \overrightarrow{\operatorname{grad}} \Phi_{j}\right)\right] d \vec{r}} \\
+\underbrace{\int_{V}^{\operatorname{grad}} \Phi_{j} \overrightarrow{\operatorname{grad}} \Phi_{i} d \vec{r}-\int_{V} \overrightarrow{\operatorname{grad}} \Phi_{i} \overrightarrow{\operatorname{grad}} \Phi_{j} d \vec{r}}_{\int_{V} S\left[\Phi_{j} \overrightarrow{\operatorname{grad}} \Phi_{i}-\Phi_{i} \overrightarrow{\operatorname{grad}} \Phi_{j}\right] d S=0}
\end{gather*}
$$

Yet

The surface integral in the equation is zero since, once more, either $\Phi_{i}$ and $\Phi_{j}$ are both zero or their gradient is zero. Finally:

$$
\left(\lambda_{i}-\lambda_{j}\right) \int_{V} \Phi_{j} \Phi_{i} d \vec{r}=0 \text { with } \lambda_{i} \neq \lambda_{j}
$$

It should be noted that this orthogonal property holds only for a bare reactor, but not for a reactor surrounded by a reflector. The eigenfunctions are known up to a constant term, and can be normalized to obtain a basis:

$$
\int_{V} \Phi_{j} \Phi_{i} d \vec{r}=1
$$

The smallest eigenvalue $\lambda_{0}$ is not degenerated and is associated to positive eigenfunction $\Phi_{0}$ over the whole volume $V$ (Planchard 1995). This particular
eigenvalue depends solely on the geometry and is called geometrical buckling. The eigenfunction associated is called the fundamental mode whereas the other functions are called the flux harmonics. These can be computed analytically for simple geometries.

### 12.2 The Notion of Geometrical and Material Buckling

The fundamental mode is the only solution such that $\Phi(r)$ is positive at all points of $V$ and $\Phi(r)=0$ for all points at the surface $S$. For any unit of the function $\Phi(r)$ (in neutron theory, it is in neutrons $/ \mathrm{cm}^{2} / \mathrm{s}$ ), the unit of $\lambda$ is the $\mathrm{cm}^{-2}$. In the case where $\lambda$ is positive, for an over-critical or critical medium, usually $\lambda=B_{g}^{2}$. where $B_{g}^{2}$ is called geometrical buckling ( $B$ for buckling and $g$ as it depends on geometry only). Geometrical buckling can be computed analytically for simple geometries and represents the radius of the flux curvature. A positive value of $\lambda$ induces a concave flux which oversees a convex domain (Fig. 12.1) whereas a negative value of $\lambda, e . g$. a source inserted in a non-multiplying medium or a sub-critical medium, leads to a convex flux shape which covers a concave domain (Fig. 12.2).

When the one-energy-group diffusion equation is written in its canonical form as $\Delta \Phi(r)+\left(k_{\infty}-1\right) \Phi(r) / M^{2}=0$, the quantity $\left(k_{\infty}-1\right) / M^{2}$ is introduced. The latter depends only on the type of multiplying medium (its isotopic composition) and not the geometry. By analogy with the purely geometric equation, $B_{m}^{2}=\left(k_{\infty}-1\right) / M^{2}$ is called material buckling when $k_{\infty}$ is larger than 1 . If $k_{\infty}$ is lower than 1 (not to be confused with the sub-criticality condition given by $k_{\text {eff }}<1$ ), the following notation $\kappa^{2}=\left(1-k_{\infty}\right) / M^{2}$ is usually employed to introduce a negative sign in the diffusion

Fig. 12.1 Example of $\lambda>0$


Fig. 12.2 Example of $\lambda<0$

equation: $\Delta \Phi(r)-\kappa^{2} \Phi(r)=0$. Coefficient $\kappa$ has the same dimensions as the inverse of length and may be taken as an attenuation coefficient. The case $k_{\infty}=1$. exists for a theoretical medium where the leakage is zero and the flux level is constant. It can only be determined mathematically by a given normalization. The set of eigenvalues of the Helmholtz equation is infinite but is still countable: $0<\lambda_{0}<\lambda_{1}<\ldots<\lambda_{n}<\ldots$, but only the fundamental mode $\Phi_{0}$ corresponding to $\lambda_{0}$ is positive at any point in the domain but is zero at its boundaries.

### 12.3 Criticality Condition

Criticality allows the existence of a stable flux in time that is positive at all points of the geometry. The following definitions are recalled:

$$
k_{e f f}=\frac{\text { production }}{\text { absorption }+ \text { leakages }}=\frac{\nu \Sigma_{f}}{\Sigma_{a}+D B_{g}^{2}} \quad \text { i.e. } \quad k_{\text {eff }}=\frac{k_{\infty}}{1+M^{2} B_{g}^{2}}
$$

which is equivalent to normalizing the production term by $k_{\text {eff }}$ in the diffusion equation:

$$
-D \Delta \Phi+\Sigma_{a} \Phi=\frac{\nu \Sigma_{f} \Phi}{k_{e f f}}
$$

The criticality condition is given simply by $k_{\text {eff }}=1$, i.e.:

$$
\begin{equation*}
\text { Criticality condition in terms of buckling: } B_{g}^{2}=\frac{k_{\infty}-1}{M^{2}} \tag{12.3}
\end{equation*}
$$

Material buckling $\left(k_{\infty}-1\right) / M^{2}$, which is dimensionally homogeneous to the inverse of a surface, corresponds to the flux curvature imposed by the properties of the medium only. Equality between material and geometrical buckling, which is a simple relation, is only of practical value if geometrical buckling can be determined analytically. This is no longer the case when the reactor geometry becomes complex, as is the case in practical situations. In this case, the criticality condition is expressed as a transcendental equation that relates the reactor geometry and the physical properties of its constituents. However, it is not possible to obtain the geometrical or material buckling from that relationship. We will consider a few practical examples below, e.g. the annular reactor.

### 12.4 Notion of Critical Size: The Rod Model

### 12.4.1 Analysis of Criticality

The classical approach of the one-dimensional rod model will be used to illustrate the notion of critical size [this proof has been established with different notations in (Wing 1962)]. Let us consider a rod of length $a$ in which neutrons move towards the right or the left.

The number of neutrons traveling at velocity $v$ in the positive direction of the $0 x$ axis is noted as $n^{+}(x)$ and $n^{-}(x)$ for the negative direction. Each neutron has a probability of being absorbed of $\Sigma_{a}(x)$ and thus, $\eta$ neutrons are produced (Fig. 12.3).

The product of $v n^{+}(x)$ corresponds to a positive current while $v n^{-}(x)$ corresponds to a negative current. For the sake of simplification, let us consider that fission is isotropic and that $\eta / 2$ neutrons are emitted to the right and the same number to the left. The neutrons may also scatter with a probability of $\Sigma_{s}(x)$. In this case, it may also be assumed that half will scatter towards the right and the others towards the left. The number of neutrons traveling to the right and undergoing collisions per second over path length $d x$ is given by:

$$
v n^{+}(x)\left[\Sigma_{a}(x)+\Sigma_{s}(x)\right] d x=v n^{+}(x) \Sigma_{t}(x) d x
$$

This equation implies that the complementary neutrons reach point $x+d x$, i.e.:

$$
\begin{equation*}
v n^{+}(x)\left[1-\Sigma_{t}(x) d x\right] \tag{12.4}
\end{equation*}
$$

Fig. 12.3 Rod geometry


From these interactions, the balance in the positive direction is:

$$
\begin{equation*}
\frac{\eta}{2} v n^{+}(x) \Sigma_{a}(x) d x+\frac{1}{2} v n^{+}(x) \Sigma_{s}(x) d x \tag{12.5}
\end{equation*}
$$

and thus, by construction, the same amount in the negative direction. Applying the same logic in the negative direction gives a number of neutrons in the positive direction produced by $n^{-}(x+d x)$, i.e.:

$$
\begin{equation*}
\frac{\eta}{2} v n^{-}(x+d x) \Sigma_{a}(x) d x+\frac{1}{2} v n^{-}(x+d x) \Sigma_{s}(x) d x \tag{12.6}
\end{equation*}
$$

According to this reasoning, the interactions due to secondary particles are not counted, and are assumed to be of second-order importance. They can be computed by applying a recurrence relation on the new amounts of secondary particles computed previously. The total number of neutrons $n^{+}(x+d x)$ is hence given at first order by the sum of Eqs. (12.4), (12.5) and (12.6):

$$
\begin{aligned}
v n^{+}(x+d x)= & v n^{+}(x)\left[1-\Sigma_{t}(x) d x\right]+\frac{\eta}{2} v n^{+}(x) \Sigma_{a}(x) d x \\
& +\frac{1}{2} v n^{+}(x) \Sigma_{s}(x) d x+\frac{\eta}{2} v n^{-}(x+d x) \Sigma_{a}(x) d x \\
& +\frac{1}{2} v n^{-}(x+d x) \Sigma_{s}(x) d x
\end{aligned}
$$

Dividing each side by $v d x$ and having the limit of $d x$ tend towards 0 , assuming that the function $n^{+}(x)$ is continuous and its derivative exists, the following equation is obtained:

$$
\begin{equation*}
\frac{d n^{+}(x)}{d x} \approx-n^{+}(x) \Sigma_{t}(x)+\frac{\eta}{2}\left[n^{+}(x)+n^{-}(x)\right] \Sigma_{a}(x)+\frac{1}{2}\left[n^{+}(x)+n^{-}(x)\right] \Sigma_{s}(x) \tag{12.7}
\end{equation*}
$$

Symmetrical logic can be applied to $n^{-}(x)$ by considering neutrons travelling to the left from $x+d x$ so as to evaluate the number of neutrons at point $x$. Hence, the following symmetrical equation is obtained:

$$
\begin{aligned}
v n^{-}(x)= & v n^{-}(x+d x)\left[1-\Sigma_{t}(x) d x\right]+\frac{\eta}{2} v n^{-}(x+d x) \Sigma_{a}(x) d x \\
& +\frac{1}{2} v n^{-}(x+d x) \Sigma_{s}(x) d x+\frac{\eta}{2} v n^{+}(x+d x) \Sigma_{a}(x) d x \\
& +\frac{1}{2} v n^{+}(x+d x) \Sigma_{s}(x) d x
\end{aligned}
$$

i.e.:
$-\frac{d n^{-}(x)}{d x}=-n^{-}(x+d x) \Sigma_{t}(x)+\frac{\eta}{2}\left[n^{+}(x)+n^{-}(x)\right] \Sigma_{a}(x)+\frac{1}{2}\left[n^{+}(x)+n^{-}(x)\right] \Sigma_{s}(x)$

By subtracting these two equations term-wise, the usual flux attenuation equation is obtained by $\Phi(x)=v\left[n^{+}(x)+n^{-}(x)\right]$, assuming that $n^{-}(x+d x) \approx n^{-}(x)$ :

$$
\frac{d \Phi(x)}{d x}=-\Sigma_{t}(x) \Phi(x)
$$

The particular case in which $\eta=2$ (which is physically realistic) and $\Sigma_{s}(x)=0$ leads to the simpler equations:

$$
\left\{\begin{array}{l}
\frac{d n^{+}(x)}{d x}=n^{-}(x) \Sigma_{a}(x) \\
\frac{d n^{-}(x)}{d x}=-n^{+}(x) \Sigma_{a}(x)
\end{array}\right.
$$

that are written in the form of a Helmholtz equation supposing a constant cross section, as:

Helmholtz equations of the absorbing rod:

$$
\begin{equation*}
\frac{d^{2} n^{+}(x)}{d x^{2}}+\Sigma_{a}^{2} n^{+}(x)=0 \quad \text { and } \quad \frac{d^{2} n^{-}(x)}{d x^{2}}+\Sigma_{a}^{2} n^{-}(x)=0 \tag{12.9}
\end{equation*}
$$

If one neutron per second is injected at the left end of the rod $(x=0)$, and assuming that there is a vacuum at both ends of the rod, any neutron leaving the rod at $x=a$ is lost and will not travel back to the right. The following boundary conditions represent that situation:

$$
\left\{\begin{array}{l}
n^{-}(a)=0 \quad \text { no neutrons reenter from the right } \\
n^{+}(0)=1
\end{array}\right. \text { neutron injected only from the left }
$$

Integrating equation (12.9) leads to the analytical solution, assuming that the cross section is constant throughout the rod:

$$
n^{+}(x)=\frac{\sin \left(\Sigma_{a}\left(x-a+\frac{\pi}{2 \Sigma_{a}}\right)\right)}{\cos \left(\Sigma_{a} a\right)} \text { and } n^{-}(x)=\frac{\cos \left(\Sigma_{a}\left(x-a+\frac{\pi}{2 \Sigma_{a}}\right)\right)}{\cos \left(\Sigma_{a} a\right)}
$$

Similar integration with the reciprocal situation where:

$$
\left\{\begin{array}{l}
n^{-}(a)=1 \text { neutron injected from the right } \\
n^{+}(0)=0 \text { no neutron reenter from the left }
\end{array}\right.
$$

leads to:

$$
n^{+}(x)=\frac{\sin \left(\Sigma_{a} x\right)}{\cos \left(\Sigma_{a} a\right)} \text { and } n^{-}(x)=\frac{\cos \left(\Sigma_{a} x\right)}{\cos \left(\Sigma_{a} a\right)}
$$

The following condition is required for these quantities to be positive:

$$
a<\frac{\pi}{2 \Sigma_{a}}
$$

Length $a=\pi /\left(2 \Sigma_{a}\right)$ leads to the rod being exactly critical, i.e. a permanent situation may be maintained in time with the imposed boundary conditions. If $a>\pi /\left(2 \Sigma_{a}\right)$, the neutron concentration $n^{+}(x)$ becomes negative over a portion of the rod, thereby leading to a physically inconsistent problem. Thus, the physical significance of the critical length is shown and will be extended in three dimensions. Let us now consider fraction $f$ of absorbed neutrons scattering in the incident direction of the absorbed neutron, and fraction $b$ scattering backwards, such that:

$$
f+b=1
$$

and, neglecting the scattering cross section for the sake of simplification, the governing equations for $n^{+}(x)$ and $n^{-}(x)$ are obtained:

$$
\left\{\begin{array}{l}
\frac{d n^{+}(x)}{d x}=n^{+}(x)[\eta f-1] \Sigma_{a}+\eta b n^{-}(x+d x) \Sigma_{a} \\
-\frac{d n^{-}(x)}{d x}=n^{-}(x)[\eta f-1] \Sigma_{a}+\eta b n^{+}(x+d x) \Sigma_{a}
\end{array}\right.
$$

This system of equations leads to the Helmholtz equation:

$$
\frac{d^{2} n^{+}(x)}{d x^{2}}+\left[\eta^{2} b^{2}-(\eta f-1)^{2}\right] \Sigma_{a}^{2} n^{+}(x)=0
$$

Applying the same boundary conditions as in the previous example, three cases are possible, depending on the sign of $\eta^{2} b^{2}-(\eta f-1)^{2}$ :

$$
\begin{array}{cl}
n^{+}(x)=\frac{\eta b \sin \left(\frac{x}{L}\right)}{\frac{1}{L \Sigma_{a}} \cos \left(\frac{a}{L}\right)-(\eta f-1) \sin \left(\frac{a}{L}\right)}, \quad L=\frac{1}{\Sigma_{a} \sqrt{\left[\eta^{2} b^{2}-(\eta f-1)^{2}\right]}}, & \eta^{2} b^{2}-(\eta f-1)^{2}>0 \\
n^{+}(x)=\frac{\eta b \operatorname{sh}\left(\frac{x}{L}\right)}{\frac{1}{L \Sigma_{a}} \operatorname{ch}\left(\frac{a}{L}\right)-(\eta f-1) \operatorname{sh}\left(\frac{a}{L}\right)}, \quad L=\frac{1}{\Sigma_{a} \sqrt{\left[(\eta f-1)^{2}-\eta^{2} b^{2}\right]}}, & \eta^{2} b^{2}-(\eta f-1)^{2}<0 \\
n^{+}(x)=\frac{\eta b \Sigma_{a} x}{1-(\eta f-1) \Sigma_{a} a}, & \eta^{2} b^{2}-(\eta f-1)^{2}=0
\end{array}
$$

In the first solution, a critical equation is reached:

$$
\frac{1}{L \Sigma_{a}} \cos \left(\Sigma_{a} \frac{a}{L}\right)-(\eta f-1) \sin \left(\Sigma_{a} \frac{a}{L}\right)=0
$$

and this may be written as follows:

$$
\begin{equation*}
\text { Criticality condition for the rod: } \tan \left(\frac{a}{L}\right)=L \Sigma_{a}(\eta f-1) \tag{12.10}
\end{equation*}
$$

The second situation leads to a criticality condition of the following form:

$$
\operatorname{th}\left(\frac{a}{L}\right)=L \Sigma_{a}(\eta f-1)
$$

It has a solution if $L \Sigma_{a}(\eta f-1)>1$. The third case leads to the following criticality equation:

$$
a=\frac{1}{(\eta f-1) \Sigma_{a}}
$$

which is physically possible only if $\eta f>1$. Some conclusions may be drawn from these results. First, criticality is never possible if $\eta<1$, and $\eta f>1$ is required to ensure the existence of critical size. For that critical size, it can easily be shown that a permanent flux solution $\Phi(x)=v\left[n^{+}(x)+n^{-}(x)\right]$ exists such that the flux is zero at both ends; this is referred to as the fundamental mode of the critical reactor.

### 12.4.2 Invariant Imbedding

(Mingle 1973; Shimizu and Aoki 1972).
Analysis of the rod model leads to the introduction of another approach called imbedding in a non-varying environment or simply the invariant imbedding approach. This technique was introduced by the astrophysicist V. A.

Ambartsumian ${ }^{3}$ in 1943, before being used by Subrahmanyan Chandrasekhar (1960). However, it was Richard Bellman ${ }^{4}$ who in 1963 named, developed and laid the generic theoretical foundations for its applications (Picture 12.2).

This method transforms a problem with two boundary conditions into an initial value problem more easily processed by computer. With the Boltzmann or diffusion equation, the flux exiting a wall subjected to incident radiation on the other side may only be obtained by first computing the complete solutions within the wall. Unlike these equations, the invariant imbedding method computes the reflection and transmission functions dependent solely on the thickness of the wall. The idea consists of computing a balance of the elementary contributions to the rate of reflected neutrons per unit time, defined by:

$$
R(x) \equiv \frac{v n^{+}(x)}{v n^{-}(x)}
$$

[^261]
(The Marguet collection)
${ }^{4}$ Ricard Ernest Bellman (1920-1984) was an American mathematician. After his studies at the Brooklyn college of the University of Wisconsin, he took part in the theoretical studies at Los Alamos on the Manhattan project. He obtained his PhD from Princeton in 1946 before teaching at Southern California University. Bellman is famous for inventing dynamic programming, an approach in the optimal control theory (Hamilton-Jacobi-Bellman equation). Bellman has published some forty books in the field of operational research and mathematics! His contribution to the nuclear field is the development of the invariant imbedding method used in radiative transfer problems. A good summary can be found in Invariant Imbedding Multipoint Boundary-Value Problems, Journal of Mathematical analysis and Applications 24, pp. 461-466 (1968).

Picture 12.2 Richard Bellman (Public domain)

Fig. 12.4 Reflection and transmission in the rod model

$R(x)$ is the number of neutrons reflected towards the right for one neutron emitted to the left.

Similarly, the transmission rate $T(x)$ is defined for one neutron emitted to the left at a distance $x$ of the considered point (Fig. 12.4).

Variation in $R(x)$ in an element $d x$ is due to at least five elementary contributions (Fig. 12.5):

$$
\begin{aligned}
R(x+d x) \equiv & \underbrace{\left(1-\Sigma_{t} d x\right) R(x)\left(1-\Sigma_{t} d x\right)}_{1}+\underbrace{c^{+} \Sigma_{t} d x}_{2}+\underbrace{c^{-} \Sigma_{t} d x R(x)\left(1-\Sigma_{t} d x\right)}_{3} \\
& +\underbrace{\left(1-\Sigma_{t} d x\right) R(x) \Sigma_{t} d x c^{+}}_{4}+\underbrace{\left(1-\Sigma_{t} d x\right) R(x) \Sigma_{t} d x c^{-} R(x)\left(1-\Sigma_{t} d x\right)}_{5}+O\left(d x^{2}\right)
\end{aligned}
$$

In this expression, $c^{+}$(respectively $c^{-}$) is the number of secondary neutrons emitted to the right (respectively to the left). In an isotropic case, $c^{+}=c^{-}$ $\equiv\left(\nu \Sigma_{f}+\Sigma_{s}\right) /\left(2 \Sigma_{t}\right)=\left(\eta \Sigma_{a}+\Sigma_{s}\right) /\left(2 \Sigma_{t}\right)$. The dependence of the cross sections in $x$ could also be easily accounted for, and would also lead to the same dependence for $c^{+}$and $c^{-}$. The first term represents the neutrons flowing in from the left and that do not interact in $d x$, each producing $R(x)$ neutrons that are reflected to the left. The other terms are deduced by similar considerations by counting the probabilities $c^{+}$ and $c^{-}$when the interaction occurs in $d x$. We have stopped at contribution 5 since

Fig. 12.5 Elementary contributions of order 1 to the reflection rate

the subsequent ones undergoing a second collision in $d x$ will be of second order (proportional to $(d x)^{2}$ ). The invariant environment term comes from the fact that the boundary condition in $x$ is always applied via the invariant albedo ${ }^{5} R(x)$. The behavior of neutrons outside the study zone is not simulated. For a more complex geometry, this approach can be generalized using leakage probabilities from one surface to the other.

By neglecting the second-order terms that are still present in the equation, the following equation is obtained (Mingle 1973, p. 14):
$\frac{R(x+d x)-R(x)}{d x}=\frac{d R(x)}{d x} \approx \Sigma_{t} c^{+}(1+R(x))-2 \Sigma_{t} R(x)+\Sigma_{t} c^{-}\left(R(x)+R^{2}(x)\right)$
with the boundary condition $R(0)=0$. This non-linear Riccati equation represents the form of the invariant environment of the rod model. Mingle notes that the same equation would be obtained by introducing $R(x)$ in Eqs. (12.7) and (12.8) and then combining them. Using the transmission rate, the differential transmission equation is written as:
$\frac{d T(x)}{d x}=2 \Sigma_{t}\left(c^{+}-1\right) T(x)+\Sigma_{t} c^{-} R(x) T(x)$ with the boundary condition $T(0)=1$

This method forms the basis of transmission theory enabling the transport equation to be solved using an original method compared to what we have seen previously. Blaquière uses a similar logic in his particle definition of the albedo

[^262](Blaquière 1962, p. 74), where this method is very effective. The invariant imbedding technique can be used in plane geometry, and though it may be extended to $l D$ cylindrical and spherical geometry, it is limited in $3 D$. In addition, flux inside the wall cannot be determined by this method. Its natural applications are in radioactive protection, where only the flux transmitted through shields is required.

### 12.5 Fundamental Mode for a Reactor with Simple Geometry

For some simple geometries, an analytical solution may be computed for the fundamental mode flux for a critical reactor. These theoretical calculations are used as verification tests for programs that can be used to handle more complex geometries. These calculations are helpful to appreciate the flux in reactors.

### 12.5.1 Plane Slab

Let us consider an infinite plane slab of thickness $a$. The one-energy group diffusion equation is simplified given that the flux no longer depends on the space variable $x$ thanks to symmetries, and is written as:

$$
\Delta \Phi(x)+\frac{k_{\infty}-1}{M^{2}} \Phi(x)=\frac{d^{2} \Phi(x)}{d x^{2}}+\frac{k_{\infty}-1}{M^{2}} \Phi(x)=0
$$

Let the characteristic equation of the case $k_{\infty}>1$ be:

$$
\frac{d^{2} \Phi}{d x^{2}}+B_{g}^{2} \Phi=0 \text { with the boundary condition: } \Phi\left(-\frac{a}{2}\right)=\Phi\left(\frac{a}{2}\right)=0
$$

The equation $d^{2} \Phi / d x^{2}-\kappa_{g}^{2} \Phi=0$ has no solution that cancels out at the boundaries of the domain. The solutions are of the form $\Phi(x)=\Phi_{\alpha} \sin \left(B_{g} x\right)$ $+\Phi_{\beta} \cos \left(B_{g} x\right)$. The solution for the flux must be symmetric, implying that $\Phi$ $(-x)=\Phi(x)$, thus $\Phi_{\alpha}=0$.

$$
\Phi\left(\frac{a}{2}\right)=\Phi\left(-\frac{a}{2}\right)=0 \quad \Rightarrow \cos \left(B_{g} \frac{a}{2}\right)=0 \quad \Rightarrow B_{g}=\frac{\pi}{a}+\frac{2 k \pi}{a} k \text { integer }
$$

The expression of the flux in the slab is deduced as:

$$
\begin{equation*}
\text { Fundamental mode of a slab: } \Phi(x)=\Phi_{\max } \cos \left(\frac{\pi}{a} x\right) \tag{12.11}
\end{equation*}
$$

Fig. 12.6 Critical slab reactor of thickness $a$


The geometrical buckling of the infinite slab of thickness $a$ is given by the formula $B_{g}^{2}=\pi^{2} / a^{2}$. Solution $B_{g}=\pi / a$ alone leads to a consistently positive-and thus the only physically acceptable-flux solution $\Phi(x)$ (Fig. 12.6).

If no further information is available, the flux is known only up to the quantity $\Phi_{\max }$. This highlights the fact that there are an infinite number of solutions to the diffusion equation. The constant $\Phi_{\max }$ can be normalized by the nuclear power produced by the slab. The case in which $k_{\infty}<1$ leads to the characteristic equation $d^{2} \Phi / d x^{2}-\kappa_{m}^{2} \Phi=0$, which has a permanent solution only if an independent neutron source buffers the system with neutrons. This is no longer the case for a critical reactor through fission, even if the sub-critical situation with a source may be encountered for an industrial reactor (during start-up for example). It may be useful to normalize the flux with the mean flux since the latter can be used to determine the power of the reactor using the formula Power $=\iiint k \Sigma_{f} \Phi d^{3} r=k \bar{\Sigma}_{f} \bar{\Phi}$. The mean flux is given by:

$$
\begin{aligned}
\bar{\Phi} & =\frac{\int_{x=-\frac{a}{2}}^{x=+\frac{a}{2}} \Phi_{\max } \cos \left(\frac{\pi}{a} x\right) d x}{\int_{x=-\frac{a}{2}}^{x=+\frac{a}{2}} d x}=\frac{\frac{a}{\pi}\left[\sin \left(\frac{\pi}{a} x\right)\right]_{x=-\frac{a}{2}}^{x=+\frac{a}{2}}}{a} \Phi_{\max } \\
& =\frac{2}{\pi} \Phi_{\max } \approx 0.637 \Phi_{\max }
\end{aligned}
$$

or, in symmetric fashion, $\Phi_{\max }=\pi \bar{\Phi} / 2$. The multiplicative coefficient of the mean flux (for instance, in the illustrative case, $\pi / 2$ ) is called form factor $\Omega$ (Lamarsh and

Barrata 2001, p. 281). A utility company would most probably seek to optimize this factor such that it is closer to 1 , either through the design of the reactor or by using an appropriate loading pattern, to avoid power peaks and ensure homogeneous fuel use-up. In practice, it is completely unrealistic to design a reactor that is critical solely by design, i.e. having a geometry that corresponds exactly to the criticality condition of the material. In addition, a critical lattice set-up could lead to a neutron flux that would be dangerous for the utility company. Thus, the reactor is designed such that it is sub-critical at loading thanks to a large reserve of mobile antireactivity (with boron in $P W R$ for example). Nevertheless, poisoning of the fuel by fission products that appear at the beginning of power production should also be taken into account, since a reactor that is only just critical at start-up could choke up by becoming sub-critical. Reactors are therefore designed to have a large reactivity reserve to be able to operate for an economically viable period, and that can be made sub-critical at start-up by adding absorbing media (boron or rods). The effective engineering problem is thus to compute the amount of absorber (boron concentration or rod position) required to turn the reactor critical for nominal operation. From a calculation point of view, the solution consists in obtaining the theoretical critical reactor for which the flux is sought such that it corresponds to a neutron source divided by a constant value, which is given by $k_{\text {eff }}$, thereby leading to:

$$
-D \Delta \Phi(x)+\Sigma_{a} \Phi(x)=\frac{\nu \Sigma_{f} \Phi}{k_{e f f}}
$$

It should be pointed out that such a reactor is a theoretical case since $k_{\text {eff }}$ is not equal to 1 , and thus, the physical flux obtained cannot be permanent and the diffusion equation should have a time-dependent term, as we will see later in the discussion of kinetics. In practical cases, the absorption cross section can be modified (by adding or subtracting boron concentrations) to calculate the $k_{\text {eff }}$ and through iteration, convergence can be reached for $k_{\text {eff }}=1$. The canonical diffusion equation is written as follows in this context:

$$
\begin{equation*}
I D \text { canonical diffusion equation: } \Delta \Phi(x)+\frac{\frac{k_{\infty}}{k_{e f f}}-1}{M^{2}} \quad \Phi(x)=0 \tag{12.12}
\end{equation*}
$$

For the case where $k_{\infty}>k_{\text {eff }}$, and by setting $B_{m}^{2} \equiv\left(k_{\infty} / k_{\text {eff }}-1\right) / M^{2}$, the eigenfunctions of the equation are $\cos (B x)$ and $\sin (B x)$. The flux solution is equal to zero at the boundary of the slab and leads to the linear system of equations as follows:

$$
\left\{\begin{array}{l}
\Phi(a / 2)=\Phi_{\alpha} \quad \sin \left(B_{m} \frac{a}{2}\right)+\Phi_{\beta} \quad \cos \left(B_{m} \frac{a}{2}\right)=0 \\
\Phi(-a / 2)=-\Phi_{\alpha} \quad \sin \left(B_{m} \frac{a}{2}\right)+\Phi_{\beta} \quad \cos \left(B_{m} \frac{a}{2}\right)=0
\end{array}\right.
$$

from which a non-trivial solution is obtained only if the determinant of the system is zero:

$$
\left|\begin{array}{cc}
\sin \left(B_{m} \frac{a}{2}\right) & \cos \left(B_{m} \frac{a}{2}\right) \\
-\sin \left(B_{m} \frac{a}{2}\right) & \cos \left(B_{m} \frac{a}{2}\right)
\end{array}\right|=0 \text { i.e.: } 2 \sin \left(B_{m} \frac{a}{2}\right) \cos \left(B_{m} \frac{a}{2}\right)=0
$$

That equation is the criticality equation from which the $k_{\text {eff }}$ of the theoretical critical reactor is obtained $B_{m} a / 2=\pi / 2$, i.e.:

$$
\frac{\frac{k_{\infty}}{k_{e f f}}-1}{M^{2}}=\left(\frac{\pi}{a}\right)^{2} \text { or even: } \quad k_{e f f}=\frac{k_{\infty}}{1+M^{2} B_{g}^{2}} \text { with } B_{g}^{2}=\left(\frac{\pi}{a}\right)^{2}
$$

If we now try to find the flux shape by imposing the boundary conditions, for instance, the flux at the boundaries of the slab (the currents could also have been set), the following is obtained:

$$
\left\{\begin{aligned}
\Phi(a / 2) & =\Phi_{\alpha} \sin \left(B_{m} \frac{a}{2}\right)+\Phi_{\beta} \cos \left(B_{m} \frac{a}{2}\right)=\Phi_{+} \\
\Phi(-a / 2) & =-\Phi_{\alpha} \sin \left(B_{m} \frac{a}{2}\right)+\Phi_{\beta} \cos \left(B_{m} \frac{a}{2}\right)=\Phi_{-}
\end{aligned}\right.
$$

The linear system of two equations with two variables leads to the solutions:

$$
\left\{\begin{array}{l}
\Phi_{\alpha}=\frac{\left(\Phi_{+}+\Phi_{-}\right) \cos \left(B_{m} \frac{a}{2}\right)}{2 \sin \left(B_{m} \frac{a}{2}\right) \cos \left(B_{m} \frac{a}{2}\right)}=\frac{\left(\Phi_{+}+\Phi_{-}\right)}{2 \sin \left(B_{m} \frac{a}{2}\right)} \\
\Phi_{\beta}=\frac{\left(\Phi_{-}-\Phi_{+}\right) \sin \left(B_{m} \frac{a}{2}\right)}{2 \sin \left(B_{m} \frac{a}{2}\right) \cos \left(B_{m} \frac{a}{2}\right)}=\frac{\left(\Phi_{-}-\Phi_{+}\right)}{2 \cos \left(B_{m} \frac{a}{2}\right)}
\end{array}\right.
$$

Since $B_{m}$ depends on $k_{e f f}$, a degree of freedom remains and can be determined by the introduction of a further equation. The latter is obtained by imposing the current at the left in the geometry, either at the right or with a flux normalization condition, e.g. by imposing the average flux value on the geometry or the flux value at a particular point in the geometry. If the maximum flux is imposed at the center, the criticality condition is written as:

$$
\Phi(0)=\Phi_{\beta}=\frac{\left(\Phi_{-}-\Phi_{+}\right)}{2 \cos \left(B_{m} \frac{a}{2}\right)}=\Phi_{\max }
$$

that is: $\left(\frac{\frac{k_{\infty}}{k_{\text {eff }}}-1}{M^{2}}\right)=\left(\frac{2}{a} \arccos \frac{\left(\Phi_{-}-\Phi_{+}\right)}{2 \Phi_{\max } \cos \left(B_{m} \frac{a}{2}\right)}\right)^{2}$
This calculation is useful to understand that the $k_{\text {eff }}$ of the theoretical critical reactor depends on the flux shape in the reactor, and that the expression $k_{\text {eff }}=k_{\infty}$ $/\left(1+M^{2} B_{g}^{2}\right)$ has a physical meaning only in the fundamental mode, i.e. the flux is zero at the boundary of the geometry. By generalizing this approach in a multigroup setting (for $G$ groups), the flux per group for the fundamental mode is expressed as a linear combination of the $2 G$ eigenfunctions, to be chosen among the 4G functions $\sin \left(\lambda_{g} x\right), \cos \left(\lambda_{g} x\right), \operatorname{sh}\left(\mu_{g} x\right), \operatorname{ch}\left(\mu_{g} x\right)$, depending on the value of $k_{\text {eff }}$ (hyperbolic functions are involved in all cases whereas trigonometric functions appear only if $k_{\text {eff }}>1$ ). There exist $G$ boundary conditions for the flux for each group, and the flux is zero at the boundaries, i.e. $2 G$ conditions. The criticality condition in the fundamental mode is then given by cancelling the determinant of the linear system with $2 G$ unknowns. The criticality condition of the critical reactor with non-zero flux at the boundaries is also obtained by adding a further equation to close the system, either by imposing the current per group at one of the boundaries or another flux value that leads to a different solution for the $k_{\text {eff }}$ and the flux shape, except for the particular case where that other value is consistent from a diffusion point of view. In reality, that situation is not really possible, especially for a code with discretized physical values. The same logic is also valid for several zones with different materials where the continuity of the flux and the currents at the interfaces is assured: one closure equation at a particular point in the geometry may be used to find the criticality condition linking the $k_{\text {eff }}$ to the materials geometry, their properties and the flux shape in the medium.

### 12.5.2 Parallelepiped

(Bonilla 1957, p. 180).
Let us consider a parallelepiped of size $a, b$ and $c$ in the directions $x, y$ and $z$. The canonical diffusion equation is written as:

$$
\Delta \Phi(x, y, z)+\frac{k_{\infty}-1}{M^{2}} \Phi(x, y, z)=\frac{\partial^{2} \Phi}{\partial x^{2}}+\frac{\partial^{2} \Phi}{\partial y^{2}}+\frac{\partial^{2} \Phi}{\partial z^{2}}+\frac{k_{\infty}-1}{M^{2}} \quad \Phi(x, y, z)=0
$$

The invariance properties thanks to the choice of the axes $x, y, z$ and the boundary conditions allow factorization of the flux as in:

$$
\Phi(x, y, z)=\phi(x) \varphi(y) \psi(z)
$$

The reader should note that if the parallelepiped were surrounded by a material, factorization would not be possible, hence the absence of a simple analytical solution even for a problem with two homogeneous media. The diffusion equation for the simple parallelepiped may be written as:

$$
\frac{\frac{d^{2} \phi(x)}{d x^{2}}}{\phi(x)}+\frac{\frac{d^{2} \varphi(y)}{d y^{2}}}{\varphi(y)}+\frac{\frac{d^{2} \psi(z)}{d z^{2}}}{\psi(z)}+\frac{k_{\infty}-1}{M^{2}}=0
$$

The sum of the functions in $x$, in $y$, in $z$ and a constant has a solution if and only if: $\frac{d^{2} \phi}{d x^{2}}+B_{x}^{2} \phi(x)=0, \frac{d^{2} \varphi}{d y^{2}}+B_{y}^{2} \varphi(y)=0$ and $\frac{d^{2} \psi}{d z^{2}}+B_{z}^{2} \psi(z)=0$
where:
Criticality condition for a parallelepiped: $B_{x}^{2}+B_{y}^{2}+B_{z}^{2}=\frac{k_{\infty}-1}{M^{2}}$
With a frame at the center of the parallelepiped, the solution is given as:

$$
\Phi(x, y, z)=\Phi_{\max } \cos \left(\frac{\pi x}{a}\right) \cos \left(\frac{\pi y}{b}\right) \cos \left(\frac{\pi z}{c}\right)
$$

The geometrical bucking for the parallelepiped is (Fig. 12.7):

$$
B_{g}^{2}=\frac{\pi^{2}}{a^{2}}+\frac{\pi^{2}}{b^{2}}+\frac{\pi^{2}}{c^{2}}
$$

Fig. 12.7 Critical parallelepiped reactor of sides $a, b, c$


The minimum volume of such a critical reactor is a cube of side $a$. The form factor is computed using a volume integral:

$$
\begin{aligned}
& x=+\frac{a}{2} \quad y=+\frac{b}{2} \quad z=+\frac{c}{2} \\
& \Phi_{\max } \int \cos \left(\frac{\pi}{a} x\right) d x \int \cos \left(\frac{\pi}{b} y\right) d y \int \cos \left(\frac{\pi}{c} z\right) d z \\
& \bar{\Phi}=\frac{x=-\frac{a}{2}}{y=-\frac{b}{2}} \quad a b c \quad z=-\frac{c}{2} \\
& =\frac{8}{\pi^{3}} \Phi_{\max } \approx 0.258 \Phi_{\max }
\end{aligned}
$$

The form factor is given by $\Omega=\pi^{3} / 8$ and is independent of the sides of the parallelepiped. It should also be pointed out that the flux in a slab is appreciably flatter than that in a cube of same side. The form factor for the parallelepiped is equal to the cube of the form factor of a slab, just as simply as a "factorization". Nevertheless, the infinite slab reactor remains a theoretical case of a finite real situation.

### 12.5.3 Infinite Cylinder

Let us consider a cylinder of radius $R$ for which the flux is sought for such that it cancels out at $R$.

$$
\left\{\begin{array}{l}
\Delta \Phi(r)+B_{g}^{2} \Phi(r)=0 \\
\Phi(R)=0
\end{array}\right.
$$

The Laplace operator in cylindrical coordinates is given as:

$$
\Delta \Phi=\frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial \Phi}{\partial r}\right)+\frac{1}{r^{2}} \frac{\partial^{2} \Phi}{\partial \theta^{2}}+\frac{\partial^{2} \Phi}{\partial z^{2}}
$$

for which only the terms in $r$ are kept thanks to the revolution symmetries. The equation may be written as follows:

$$
r^{2} \frac{d^{2} \Phi(r)}{d r^{2}}+r \frac{d \Phi(r)}{d r}+B_{g}^{2} r^{2} \Phi(r)=0
$$

This is in fact the Bessel equation ${ }^{6}$ with the addition of the term $B_{g}^{2}$ (Hochstadt 1973, p. 180). Variable $\rho=B_{g} r$ may be changed so as to obtain a canonical Bessel equation. ${ }^{7}$ The general solution of this modified Bessel equation is usually:

$$
\Phi(r)=\Phi_{J} J_{0}\left(B_{g} r\right)+\Phi_{Y} Y_{0}\left(B_{g} r\right)
$$

The flux $\Phi(r)$ must be finite $\left(=\Phi_{\max }\right)$; since as $Y_{0}(0)=-\infty, \Phi_{Y}=0$. The boundary condition enabling the flux to be equal to zero on the surface of the cylinder is given by $\Phi(R)=0$, i.e. $J_{0}\left(B_{g} R\right)=0$. Hence, $B_{g} R$ is the square root of the function $J_{0}$ (usually denoted as $j_{0, k}$ i.e. the $k^{i t h}$ root of the function $J_{0}$ ) and only the first root ensures that the flux is positive at any point in the cylinder. Since $J_{0}(0)=1$, the solutions to the Helmholtz equation are given as (Fig. 12.8):

$$
\Phi_{n}(r)=\Phi_{\max } J_{0} \quad\left(j_{0, n} r / R\right)
$$

Only $\Phi_{1}(r)$ is positive at any point. The geometrical buckling for an infinite cylinder is:

[^263]
(The Marguet collection)
${ }^{7}$ For further explanations on the Bessel functions, see (Watson 1980).

Fig. 12.8 Cylindrical reactor of radius $R$


$$
B_{g}^{2}=\left(\frac{j_{0,1}}{R}\right)^{2} \approx\left(\frac{2.405}{R}\right)^{2}
$$

The average flux is given by the following equation:

$$
\bar{\Phi}=\frac{\int_{r=0}^{r=+R} \Phi_{\max } J_{0}\left(\frac{j_{0,1} r}{R}\right) 2 \pi r d r}{\int_{r=0}^{r=+R} 2 \pi r d r}=\frac{2 \pi\left(\frac{R}{j_{0,1}}\right)^{2} \int_{r=0}^{r=+R} \frac{j_{0,1} r}{R} J_{0}\left(\frac{j_{0,1} r}{R}\right) \frac{j_{0,1}}{R} d r}{\pi R^{2}} \Phi_{\max }
$$

Using the formula for an integral of $x J_{0}(x)$ :

$$
\begin{aligned}
& \qquad \begin{aligned}
\int_{r=0}^{r=+R} \frac{j_{0,1} r}{R} J_{0}\left(\frac{j_{0,1} r}{R}\right) \frac{j_{0,1}}{R} d r & =\int_{x=0}^{x=+j_{0,1}} x J_{0}(x) d x=\left[x J_{1}(x)\right]_{x=0}^{x=+j_{0,1}} \\
& =j_{0,1} J_{1}\left(j_{0,1}\right)
\end{aligned} \\
& \text { i.e. }: \bar{\Phi}=\frac{2 \pi\left(\frac{R}{j_{0,1}}\right)^{2} j_{0,1} J_{1}\left(j_{0,1}\right)}{\pi R^{2}} \Phi_{\max }=\frac{2 J_{1}\left(j_{0,1}\right)}{j_{0,1}} \Phi_{\max } \approx 0.416 \Phi_{\max }
\end{aligned}
$$

with $j_{0,1} \approx 2.405$ and $J_{1}\left(j_{0,1}\right) \approx 0.5$. The form factor for the infinite cylinder is thus $\Omega=\frac{j_{0,1}}{2 J_{1}\left(j_{0,1}\right)}$.

### 12.5.4 Finite Cylinder

(Cameron 1982, p. 97).
Let us consider a finite reactor of radius $R$ and height $H$.

$$
\Delta \Phi(r, z)+B_{g}^{2} \Phi(r, z)=\frac{\partial^{2} \Phi(r, z)}{\partial r^{2}}+\frac{1}{r} \frac{\partial \Phi(r, z)}{\partial r}+\frac{\partial^{2} \Phi(r, z)}{\partial z^{2}}+B_{g}^{2} \Phi(r, z)=0
$$

Thanks to this geometry, a solution may be obtained by separating the variables $\Phi(r, z)=\varphi(r) \psi(z)$ and the diffusion equation is written as:

$$
\underbrace{\frac{1}{\varphi(r)} \frac{d^{2} \varphi(r)}{d r^{2}}+\frac{1}{\varphi(r) r} \frac{d \varphi(r)}{d r}}_{\text {Depends only on } r}+\underbrace{\frac{1}{\psi(z)} \frac{d^{2} \psi(z)}{d z^{2}}+B_{g}^{2}}_{\text {Depends only on } z}=0
$$

This equation is possible if:

$$
\frac{1}{\varphi(r)} \frac{d^{2} \varphi(r)}{d r^{2}}+\frac{1}{\varphi(r)} \frac{d \varphi(r)}{d r}=A, \frac{1}{\psi(z)} \frac{d^{2} \psi(z)}{d z}=C, A+C+B_{g}^{2}=0
$$

where $A$ and $C$ are constants. A physical solution that is equal to zero at $z=+H / 2$ and $z=-H / 2$ requires that $C \leq 0$. Hence:

$$
\frac{1}{\Psi_{(z)}} \frac{d^{2} \Psi_{(z)}}{d z^{2}}=-\alpha^{2}
$$

The equation for a slab of thickness $H$ is $\psi(z)=\psi_{1 \max } \cos (\pi z / H)$.

$$
\text { where : } \quad A=-B_{g}^{2}-C=-B_{g}^{2}+\left(\frac{\pi}{H}\right)^{2}
$$

Hence:

$$
\frac{d^{2} \varphi(r)}{d r^{2}}+\frac{1}{r} \frac{d \varphi(r)}{d r}+\underbrace{\left(B_{g}^{2}-\frac{\pi^{2}}{H^{2}}\right)}_{\beta^{2}} \varphi(r)=0
$$

This zero-order Bessel equation has the general solution: $\varphi_{J} J_{0}(\beta r)+\varphi_{Y} Y_{0}(\beta r)$. Similar logic as for the case of the infinite cylinder leads to elimination of the function $Y_{0}(\beta r)$, which is equal to $-\infty$ at 0 . Since $\varphi(\beta R)=0$, it may be deduced that: $\beta R=j_{0,1}$ (Fig. 12.9).

Only the first root $j_{0,1}$ ensures a positive flux $\varphi(r)$. Therefore:

$$
\varphi(r)=\varphi_{1_{\max }} J_{0}\left(j_{0,1} r / R\right)
$$

Fig. 12.9 Critical cylindrical reactor


Thus, the complete flux solution is reached by recalling that $\Phi(r, z)=\varphi(r) \psi(z)$ and that $j_{0,1} \approx 2.405$.

$$
\Phi(r, z)=\Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R} r\right) \cos \left(\pi \frac{z}{H}\right)
$$

The geometrical buckling of a finite cylinder is given by:

$$
B_{g}^{2}=\left(\frac{j_{0,1}}{R}\right)^{2}+\left(\frac{\pi}{H}\right)^{2}
$$

Therefore, the solution of the critical equation for the finite cylinder as expressed by:

$$
-D \Delta \Phi(r, z)+\Sigma_{a} \Phi(r, z)=\frac{\nu \Sigma_{f} \Phi(r, z)}{k_{e f f}}
$$

is similar to that obtained for an infinite cylinder with a flux solution $\Phi(r)$ where the leakage term $D B_{z}^{2}=D\left(\pi^{2} / H^{2}\right)$ is added to the absorption:

$$
-D \Delta \Phi(r)+\left[\Sigma_{a}+D B_{z}^{2}\right] \Phi(r)=\frac{\nu \Sigma_{f} \Phi(r)}{k_{e f f}}
$$

since $\cos \left(B_{z} z\right)$, which represents the flux component in the calculations in two dimensions $(r, z)$, is the eigenfunction of the equation in $z$ which is obtained by setting $\Phi(r, z)=\phi(r) \varphi(z)$ :

$$
-\frac{\partial^{2} \varphi(z)}{\partial z^{2}}=B_{z}^{2} \varphi(z)
$$

Amongst other advantages, this approach allows simple calculation of the loading pattern of the core in three dimensions using a two-dimensional calculation ( $x O y$ plane) by including the axial leakage term $D B_{z}^{2}$ to the absorption. In other words, the flux is assumed to be the fundamental mode. Similarly, an $1 D$ axial calculation may be made more representative by introducing a leakage term to the absorption. This approach may be improved by introducing a radial leakage term for each layer of $1 D$ core or axial leakage for each $2 D$ assembly, without obtaining the accuracy of a true $3 D$ calculation. The flux can be expressed in terms of the mean flux by computing the dependence of the latter with respect to the maximum flux using a triple integration (volume integration) over the volume of the cylinder:

$$
\begin{aligned}
\bar{\Phi} & =\frac{\int_{r=0}^{r=R} \int_{\theta=0}^{\theta=2 \pi} \int_{z=-\frac{H}{2}}^{z=+\frac{H}{2}} \Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R} r\right) \cos \left(\frac{\pi z}{H}\right) d z r d \theta d r}{r=R} \int_{r=0} \int_{\theta=0} \int_{z=-\frac{H}{2}}^{z=+\frac{H}{2}} d z r d \theta d r \\
& =\Phi_{\max } \frac{2 \pi \frac{2 H}{\pi} \int_{r=0}^{r=R} J_{0}\left(\frac{j_{0,1}}{R} r\right) r d r}{\pi R^{2} H}
\end{aligned}
$$

Using the following integration formula: $\int r J_{0}(r) d r=r J_{1}(r)$ and the change in variable $x=j_{0,1} r / R$ :

$$
\bar{\Phi}=\Phi_{\max } \frac{4}{\pi R^{2}} \frac{R^{2}}{j_{0,1}^{2}} \int_{r=0}^{r=R} \frac{j_{0,1}}{R} r J_{0}\left(\frac{j_{0,1}}{R} r\right) \frac{j_{0,1}}{R} d r=\Phi_{\max } \frac{4}{\pi j_{0,1}} J_{1}\left(j_{0,1}\right) \approx 0.265 \Phi_{\max }
$$

The form factor obtained is $\Omega=\frac{\pi j_{0,1}}{4 J_{1}\left(j_{0,1}\right)}$,i.e. the product of the form factor of a slab and an infinite cylinder.

### 12.5.5 Disc

Let us consider a disc in two dimensions $(r, \theta)$ with $r<R$ the radius of the disc, with constant properties, but nevertheless with a boundary condition applied to its edge depending on the angle. The diffusion equation in cylindrical coordinates is written as:

$$
-D\left[\frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial \Phi(r, \theta)}{\partial r}\right)+\frac{1}{r^{2}} \frac{\partial^{2} \Phi(r, \theta)}{\partial \theta^{2}}\right]+\Sigma_{a} \Phi(r, \theta)=\frac{\nu \Sigma_{f} \Phi(r, \theta)}{k_{e f f}}
$$

It is very effective to expand the flux as an infinite series of Chebychev polynomials $T_{l}(\theta) \equiv \cos (l \theta)$ (i.e. Fourier series), discussed earlier in the $T_{n}$ form of the Boltzmann equation:

$$
\Phi(r, \theta)=\sum_{l=0}^{\infty} \Phi_{l}(r) T_{l}(\theta)
$$

The second derivative of a Chebychev polynomial is:

$$
\frac{\partial^{2} T_{l}(\theta)}{\partial \theta^{2}}=-l^{2} T_{l}(\theta)
$$

Using flux expansion in the diffusion equation, the following equation is obtained:
with the expression of material buckling:

$$
B_{m}^{2}=\frac{\nu \Sigma_{f}}{D k_{e f f}}-\frac{\Sigma_{a}}{D} \text { if } \Sigma_{a}<\frac{\nu \Sigma_{f}}{k_{e f f}}
$$

corresponding to a disc with positive neutron leakage and

$$
\kappa^{2}=\frac{\Sigma_{a}}{D}-\frac{\nu \Sigma_{f}}{D k_{e f f}} \text { if } \Sigma_{a}>\frac{\nu \Sigma_{f}}{k_{e f f}}
$$

i.e. neutrons entering through the external surface of the disc, thereby explaining the $\pm$ sign in the equation. The orthogonality properties of the Chebychev polynomials are then used:

$$
\int_{-1}^{+1} \frac{T_{n}(\mu) T_{m}(\mu)}{\sqrt{1-\mu^{2}}} d \mu= \begin{cases}0 & \text { if } n \neq m \\ \pi & \text { if } n=m=0 \\ \frac{\pi}{2} & \text { if } n=m \neq 0\end{cases}
$$

multiplying the equation by $T_{l}(\mu) / \sqrt{1-\mu^{2}}$ for all values of $l$ and integrating over $\mu=\cos \theta \in[-1,1]$ to obtain the equation with the flux moments:

$$
\frac{\partial^{2} \Phi_{l}(r)}{\partial r^{2}}+\frac{1}{r} \frac{\partial \Phi_{l}(r)}{\partial r}-\left(l^{2}+\left\{\begin{array}{l}
-B_{m}^{2} \\
+\kappa_{m}^{2}
\end{array}\right) \Phi_{l}(r)=0\right.
$$

It can be seen that this is a Bessel equation when it is written with the term $l^{2}-B_{m}^{2}$, and for which the general solution is $\alpha J_{l}\left(B_{m} r\right)+\beta Y_{l}\left(B_{m} r\right)$, and a modified Bessel equation when written with $l^{2}+\kappa_{m}^{2}$, with $\gamma I_{l}\left(B_{m} r\right)+\delta K_{l}\left(B_{m} r\right)$ being the solution. The specific case where $B_{m}^{2}=0$, i.e. $\Sigma_{a}=\nu \Sigma_{f} / k_{e f f}$ (no leakage) has a solution of the form $\lambda r^{l}+\varpi r^{-l}$ if $l \neq 0$, and $\vartheta \log (r)+\tau$ if $l=0$. The fact that the flux has a finite value at $r=0$ leads to zero coefficients for $\beta=\delta=\omega=\vartheta=0$, thereby restricting the solutions to:

$$
\Phi_{l}(r)=\left\{\begin{array}{lll}
I_{l}\left(\kappa_{m} r\right) & \text { for } & \kappa_{m}>0 \quad l \neq 0 \\
J_{l}\left(B_{m} r\right) & \text { for } \quad B_{m}>0 & l \neq 0 \\
r^{l} & \text { for } B_{m}=0 &
\end{array}\right.
$$

The other coefficients may be determined according to the boundary condition, and denoted as $\alpha_{l}$. For a Dirichlet condition:

$$
\Phi(R, \theta)=\Psi(\theta)=\sum_{l=0}^{\infty} \alpha_{l} \Phi_{l}(R) T_{l}(\theta)
$$

the coefficient $\alpha_{l}$ is obtained using the following orthogonality relation:

$$
\left\{\begin{array}{l}
\alpha_{0}=\frac{1}{\pi \Phi_{0}(R)} \int_{-1}^{+1} \frac{\Psi(\mu)}{\sqrt{1-\mu^{2}}} d \mu \\
\alpha_{l}=\frac{2}{\pi \Phi_{l}(R)} \int_{-1}^{+1} \frac{T_{l}(\mu) \Psi(\mu)}{\sqrt{1-\mu^{2}}} d \mu
\end{array}\right.
$$

For Neumann boundary conditions ${ }^{8}$ :

$$
\left.\frac{\partial \Phi(r, \theta)}{\partial r}\right|_{R}=\Phi(\theta)=\left.\sum_{l=0}^{\infty} \alpha_{l} \frac{d \Phi_{l}(r)}{d r}\right|_{R} T_{l}(\theta) .
$$

the derivatives of the Bessel functions of the first kind may be computed using the following relations:

$$
\begin{cases}\frac{d J_{l}\left(B_{m} r\right)}{d r}=B_{m} \frac{J_{l-1}\left(B_{m} r\right)-J_{l+1}\left(B_{m} r\right)}{2} & \frac{d J_{0}\left(B_{m} r\right)}{d r}=-B_{m} J_{1}\left(B_{m} r\right) \\ \frac{d I_{l}\left(\kappa_{m} r\right)}{d r}=\kappa_{m} \frac{I_{l-1}\left(\kappa_{m} r\right)+I_{l+1}\left(\kappa_{m} r\right)}{2} & \frac{d I_{0}\left(\kappa_{m} r\right)}{d r}=\kappa_{m} I_{1}\left(\kappa_{m} r\right)\end{cases}
$$

[^264]Thus, by conditioning similar to a Dirichlet condition:

$$
\left\{\begin{array}{l}
\alpha_{0}=-\frac{1}{\pi B_{m} J_{1}\left(B_{m} R\right)} \int_{-1}^{+1} \frac{\Phi(\mu)}{\sqrt{1-\mu^{2}}} d \mu \\
\alpha_{l}=\frac{4}{\pi B_{m}\left(J_{l-1}\left(B_{m} R\right)-J_{l+1}\left(B_{m} R\right)\right)} \int_{-1}^{+1} \frac{T_{l}(\mu) \Phi(\mu)}{\sqrt{1-\mu^{2}}} d \mu
\end{array}\right.
$$

or even:

$$
\left\{\begin{array}{l}
\alpha_{0}=\frac{1}{\pi \kappa_{m} I_{1}\left(\kappa_{m} R\right)} \int_{-1}^{+1} \frac{\Phi(\mu)}{\sqrt{1-\mu^{2}}} d \mu \\
\alpha_{l}=\frac{4}{\pi \kappa_{m}\left(I_{l-1}\left(\kappa_{m} R\right)+I_{l+1}\left(\kappa_{m} R\right)\right)} \int_{-1}^{+1} \frac{T_{l}(\mu) \Phi(\mu)}{\sqrt{1-\mu^{2}}} d \mu
\end{array}\right.
$$

A boundary condition of Robin type:

$$
\Phi(R, \theta)+\left.\lambda \frac{\partial \Phi(r, \theta)}{\partial r}\right|_{R}=\varphi(\theta)
$$

may be considered by mixing both previous approaches.

### 12.5.6 Sphere

The diffusion equation is written as follows in spherical coordinates:

$$
\Delta \Phi(r, \theta, \varphi)+B_{g}^{2} \Phi(r, \theta, \varphi)=0
$$

The Laplace operator in spherical coordinates is recalled as:

$$
\Delta \Phi=\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial \Phi}{\partial r}\right)+\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial \Phi}{\partial \theta}\right)+\frac{1}{r^{2} \sin ^{2} \theta} \frac{\partial^{2} \Phi}{\partial \varphi^{2}}
$$

This equation has a positive mathematical solution that cancels out at the boundaries of the reactor. This solution is expressed in terms of spherical harmonics $Y_{n m}(\theta, \varphi)$ and spherical Bessel functions $j_{n}(r)$ (the terms in $y_{n}(r)$, the second spherical Bessel function, disappear when $y_{n}(r)$ tends towards $-\infty$ as $r$ tends towards 0).

$$
\begin{gathered}
\Phi_{n}(r, \theta, \varphi)=\left\{\begin{array}{cl}
j_{0}\left(B_{g} r\right)=\frac{\sin \left(B_{g} r\right)}{B_{g} r} & n=0 \\
j_{n}\left(B_{g} r\right) \sum_{m=0}^{n} Y_{n m}(\theta, \varphi) & n \geq 1
\end{array}\right. \\
\text { with }: j_{n}\left(B_{g} r\right)=\left\{\begin{array}{cc}
\frac{\sin \left(B_{g} r\right)}{B_{g} r} & n=0 \\
\left(B_{g} r\right)^{n}\left(-\frac{1}{B_{g} r d\left(B_{g} r\right)}\right)^{n} \frac{\sin \left(B_{g} r\right)}{B_{g} r} & n \geq 1
\end{array}\right.
\end{gathered}
$$

The spherical Bessel functions $j_{n}(r)$ satisfy the equation:

$$
r^{2} \frac{d^{2} j_{n}(r)}{d r^{2}}+2 r \frac{d j_{n}(r)}{d r}+\left[r^{2}-n(n+1)\right] j_{n}(r)=0
$$

For a homogeneous sphere of radius $R$, the spherical symmetry of the flux eliminates the dependence at angles $\theta$ and $\varphi$ :

$$
\left\{\begin{array}{l}
\Delta \Phi(r)+B_{g}^{2} \Phi(r)=\frac{d^{2} \Phi(r)}{d r^{2}}+\frac{2}{r} \frac{d \Phi(r)}{d r}+B_{g}^{2} \Phi(r)=0 \\
\Phi(R)=0 \text { and } \Phi(0)=\Phi_{\max }
\end{array}\right.
$$

The solution to this problem can be obtained without any particular knowledge of the spherical Bessel functions. A variable change with $\varphi(r)=r \Phi(r)$ leads to:

$$
\left\{\begin{array}{c}
\frac{d^{2} \varphi(r)}{d r^{2}}+\lambda \varphi(r)=0 \\
\varphi(0)=\varphi(R)=0
\end{array}\right.
$$

This is the same equation as that obtained for the plane slab geometry, and for which only the sine function solution is kept since $\varphi(0)=0$. Thus, $\varphi(r)=\varphi_{1_{\max }} \sin (\pi r / R)$.

Hence:

$$
\Phi(r)=\varphi_{1_{\max }} \frac{\sin \left(\frac{\pi}{R} r\right)}{r}
$$

The following equation is employed to evaluate the maximum flux at the center of the sphere:

$$
\Phi_{\max }=\lim _{r \rightarrow 0} \Phi(r)=\varphi_{1_{\max }} \lim _{r \rightarrow 0} \frac{\sin \left(\frac{\pi}{R} r\right)}{r}=\varphi_{1_{\max }} \frac{\pi}{R} \lim _{r \rightarrow 0} \frac{\sin \left(\frac{\pi}{R} r\right)}{\frac{\pi}{R} r}=\phi_{1_{\max }} \frac{\pi}{R}
$$

Fig. 12.10 Critical
spherical reactor of radius $R$


The solution obtained is of the form of a spherical Bessel function $j_{0}\left(B_{g} r\right)$ :

$$
\Phi(r)=\Phi_{\max } \frac{\sin \left(\frac{\pi}{R} r\right)}{\frac{\pi}{R} r}
$$

The geometrical buckling of a sphere of radius R is expressed as (Fig. 12.10):

$$
B_{g}^{2}=\left(\frac{\pi}{R}\right)^{2}
$$

The flux is expressed in terms of the mean flux by computing the mean flux with respect to the maximum flux using a volume integral for the sphere:

$$
\begin{aligned}
& \bar{\Phi}=\frac{\int_{r=0}^{r=R} \int_{\theta=0}^{\theta=2 \pi} \int_{\varphi=0}^{\varphi=\pi} \Phi_{\max } \frac{R \sin \left(\frac{\pi}{R} r\right.}{\pi r}}{} r^{2} \sin \varphi d \varphi d \theta d r \\
& \int_{r=0}^{r=R} \int_{\theta=0}^{\theta=2 \pi} \int_{\varphi=0}^{\varphi=\pi} r^{2} \sin \varphi d \varphi d \theta d r \\
&=\Phi_{\max } \frac{R}{\pi} \frac{\int_{r=0}^{r=R} \sin \left(\frac{\pi}{R} r\right) r d r \int_{\theta=0}^{\theta=2 \pi} d \theta \int_{\varphi=0}^{\varphi=\pi} \sin \varphi d \varphi}{\frac{4}{3} \pi R^{3}}
\end{aligned}
$$

using the following change in variable: $x=\pi r / R$. The mean flux results from an integration by parts:

$$
\bar{\Phi}=\Phi_{\max } \frac{R^{3}}{\pi^{3}} \frac{4 \pi \int_{x=0}^{x=\pi} x \sin x d x}{\frac{4}{3} \pi R^{3}}=\frac{3}{\pi^{2}} \Phi_{\max } \approx 0.304 \Phi_{\max }
$$

The form factor for a sphere is thus $\Omega=\pi^{2} / 3$. The sphere is the geometrical shape having the smallest critical volume since it has the smallest surface to volume ratio, thereby reducing leakage. Price et al. (1957, p. 166) proposes several solutions for spherical geometries with distributed sources.

### 12.5.7 Hemisphere

The case of the hemisphere with null flux at its surface (for both the spherical and plane surfaces) requires a fundamental mode solution that depends on the angle $\theta-$ the flux in a homogeneous sphere depends only on $r$ and cannot be employed. The two-dimensional spherical harmonics $Y_{n m}(\theta, \varphi)$ simplify into the first-order Legendre polynomial $P_{1}(\cos \theta)=\cos \theta$ and the flux is obtained as:

$$
\Phi(r, \theta)=j_{1}\left(B_{g} r\right) \quad Y_{1}(\theta)=\left[\frac{\sin \left(B_{g} r\right)}{\left(B_{g} r\right)^{2}}-\frac{\cos \left(B_{g} r\right)}{B_{g} r}\right] \cos \theta
$$

By the very definition of $j_{1}\left(B_{g} r\right)$, the flux is zero at $r=0$. It remains null for any angle $\theta$ at $r=R$ if $j_{1}\left(B_{g} R\right)=0$, i.e. when $B_{g} R$ is the first non-zero root of the spherical Bessel function $j_{1}(r)$, for $j_{1,1}^{s}=4.4934$. The geometrical buckling of a hemisphere is thus:

$$
B_{g}^{2}=\frac{j_{1,1}^{s}}{R^{2}} \approx \frac{4.4934}{R^{2}}
$$

It is worth mentioning that ${ }^{9}$ the criticality equation for a hemisphere:

$$
-D\left[\frac{1}{r^{2}} \frac{\partial}{\partial}\left(r^{2} \frac{\partial \Phi}{\partial r}\right)+\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial \Phi}{\partial \theta}\right)\right]+\Sigma_{a} \Phi=\frac{\nu \Sigma_{f} \Phi}{k_{e f f}}
$$

may be simplified to:

$$
-D\left[\frac{1}{r^{2}} \frac{\partial}{\partial}\left(r^{2} \frac{\partial \Phi}{\partial r}\right)\right]+\left(\Sigma_{a}+D B^{2}(r)\right) \Phi=\frac{\nu \Sigma_{f} \Phi}{k_{e f f}} \text { with } B^{2}(r)=\frac{2}{r^{2}}
$$

if $\cos \theta$, which represents the angular component of the flux, is the eigenfunction of:

[^265]Fig. 12.11 Hexagon and its circumscribed and inscribed circles


$$
-\left[\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial \Phi}{\partial \theta}\right)\right]=B^{2}(r) \Phi=\frac{2}{r^{2}} \Phi
$$

This implies that the flux calculation for a hemispherical geometry may be evaluated with a $l D$ radial computation using a leakage correction term $D B^{2}(r)$ that is added to absorption.

### 12.5.8 Polygon

A recent study ${ }^{10}$ has enabled determination of the geometrical buckling for regular polygons with both numerical and experimental validation. The starting-point for the method is to express the geometrical buckling of an $n$-sided polygon in the form $a_{n}^{2} / R_{c}^{2}$, with $R_{c}$ being the radius of the circumscribed circle. With $R_{i}$ as the radius of the inscribed circle, it may be readily seen that, geometrically, the buckling of the polygon is bounded by that of the circumscribed and inscribed circles (Fig. 12.11):

$$
\frac{j_{0,1}^{2}}{R_{c}^{2}} \leq \frac{a_{n}^{2}}{R_{c}^{2}} \leq \frac{j_{0,1}^{2}}{R_{i}^{2}}
$$

However, the fact that buckling of a polygon is greater than that of a circle of the same surface area seems less obvious:

$$
A_{n}=\frac{n R_{c}^{2}}{2} \sin \left(\frac{2 \pi}{n}\right)
$$

[^266]$$
\text { If : } \frac{\pi j_{0,1}^{2}}{\frac{n R_{c}^{2}}{2} \sin \left(\frac{2 \pi}{n}\right)} \leq \frac{a_{n}^{2}}{R_{c}^{2}}
$$

Given that $R_{i}=R_{c} \cos \left(\frac{\pi}{n}\right), a_{n}$ is bounded by two series as given below:

$$
\frac{\pi j_{0,1}^{2}}{\frac{n}{2} \sin \left(\frac{2 \pi}{n}\right)} \leq a_{n}^{2} \leq \frac{j_{0,1}^{2}}{\cos ^{2}\left(\frac{\pi}{n}\right)}
$$

For the hexagon in the above example, the numerical values are $2.644 \leq a_{n} \leq 2.777$, and these must be compared to the limit $j_{0,1}=2.405$, which is the buckling of a disc. Obtaining the geometrical buckling of a polygon is important because if the whole space is paved with these polygons, the Wielandt algorithm (Wachspress 1966, p. 20), can be employed efficiently. This algorithm consists in accelerating the external iterations (indexed by $m$ ) of a diffusion calculation using an estimator, $\lambda_{W}$, of the $k_{\text {eff }}{ }^{11}$ :

[^267]

Helmut Wielandt (University of Berlin)

$$
\left\{\begin{array}{l}
-D \Delta \Phi^{m}+\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{\lambda_{W}}\right) \Phi^{m}=\left(\frac{1}{k_{e f f}^{m-1}}-\frac{1}{\lambda_{W}}\right) \nu \Sigma_{f} \Phi^{m-1} \\
\frac{\nu \Sigma_{f}}{\lambda_{W}}-\Sigma_{a}>0
\end{array}\right.
$$

Thus, by choosing $\lambda_{W}=\frac{\nu \Sigma_{f}}{\Sigma_{a}+D B_{g}^{2}}$ with $B_{g}^{2}=\frac{1}{2}\left[\frac{\pi j_{0,1}^{2}}{\frac{n}{2} \sin \left(\frac{2 \pi}{n}\right)}+\frac{j_{0,1}^{2}}{\cos ^{2}\left(\frac{\pi}{n}\right)}\right]$, convergence may be significantly accelerated.

### 12.5.9 Accounting for Singularities in 2D

The corners of $2 D$ geometries lead to singularities that pose analytical difficulties in diffusion theory. In a mono-energy approach, the diffusion equation for a domain formed by two homogeneous sub-domains $\Omega=\Omega_{1} \cup \Omega_{2}$ is written as:

$$
\left\{\begin{array}{l}
-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi(r, \theta))+\Sigma_{t} \Phi(r, \theta)=S \quad \text { in } \Omega \\
\Phi(r, \theta)=0 \quad \text { over } \partial \Omega
\end{array}\right.
$$

The required solution to this problem should (Fig. 12.12):

- cancel out at the boundary of the domain,
- be continuous at the interface $\Gamma$ that separates the domains,
- lead to a singularity.

Let $\Omega_{0}=\{0 \leq r \leq R, 0 \leq \theta \leq 2 \pi\}$ be a disc, with its center at the singularity, $O$. The strategy consists in expanding the flux as follows:

$$
\Phi(r, \theta)=\sum_{l=0}^{\infty} \Phi_{l}(r) \varphi_{l}(\theta)
$$

where $\varphi_{l}(\theta)$ is the continuous solution to the Sturm-Liouville problem at the interface $\Gamma$ :

Fig. 12.12 Singularity between two homogeneous domains


$$
\left\{\begin{array}{l}
\frac{d\left(D(\theta) \frac{d \varphi(\theta)}{d \theta}\right)}{d \theta}+\mu^{2} D(\theta) \varphi(\theta)=0 \quad \text { in } \Omega \\
\left.D(\theta) \frac{d \varphi(\theta)}{d \theta}\right|_{\theta_{\Gamma}^{+}}=\left.D(\theta) \frac{d \varphi(\theta)}{d \theta}\right|_{\theta_{\Gamma}^{-}} \\
\varphi\left(\theta_{\Gamma}^{+}\right)=\varphi\left(\theta_{\Gamma}^{-}\right) \quad \text { and } \quad \varphi\left(0^{+}\right)=\varphi\left(0^{-}\right)
\end{array}\right.
$$

It can be proven mathematically ${ }^{12}$ that the solution to this self-adjoint problem is a sequence of positive eigenvalues, with associated eigenfunctions $\varphi_{l}(\theta)$ that are orthogonal on the $L^{2}([O, 2 \pi])$ space. These functions satisfy the following orthogonality relation:

$$
\left\{\begin{array}{l}
\int_{0}^{2 \pi} D(\theta) \varphi_{n}(\theta) \varphi_{m}(\theta) d \theta=\delta_{n, m} \\
\int_{0}^{2 \pi} D(\theta) \frac{d \varphi_{n}(\theta)}{d \theta} \frac{d \varphi_{m}(\theta)}{d \theta} d \theta=\mu_{m}^{2} \delta_{n, m}
\end{array}\right.
$$

The variational formulation for the diffusion problem is expressed so as to determine the spatial flux moments:

$$
F[\Psi]=\int_{\Omega}\left(-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi(r, \theta))+\Sigma_{t} \Phi(r, \theta)\right) \Psi(r, \theta) d^{2} \Omega-\int_{\Omega} S \Psi(r, \theta) d^{2} \Omega
$$

The goal is to cancel out the functional by choosing the function $\Psi(r, \theta)$, which is zero everywhere save on the disc $\Omega_{0}$. Using:

$$
\begin{aligned}
\Psi(r, \theta) \operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi(r, \theta))= & \operatorname{div}(\Psi(r, \theta) D \overrightarrow{\operatorname{grad}} \Phi(r, \theta)) \\
& -D \overrightarrow{\operatorname{grad}} \Phi(r, \theta) \cdot \overrightarrow{\operatorname{grad}} \Psi(r, \theta)
\end{aligned}
$$

then, by applying the Ostrogradski theorem:

$$
\int_{\Omega} \operatorname{div}(\Psi(r, \theta) D \overrightarrow{\operatorname{grad}} \Phi(r, \theta)) d^{2} \Omega=\int_{\partial \Omega} \Psi(r, \theta) D \overrightarrow{\operatorname{grad}} \Phi(r, \theta) d \Omega=0
$$

[^268]The variational formulation thus obtained is limited to the disc (since $\Psi$ is zero elsewhere):

$$
\int_{\Omega_{0}}\left(D \overrightarrow{\operatorname{grad}} \Phi(r, \theta) \cdot \overrightarrow{\operatorname{grad}} \Psi(r, \theta)+\Sigma_{t} \Phi(r, \theta)\right) \Psi(r, \theta) d^{2} \Omega=\int_{\Omega_{0}} S \Psi(r, \theta) d^{2} \Omega
$$

The trial function is set using the separation of variables principle and a Heaviside function to cancel it outside the disc and with a particular function of order $m$ :

$$
\Psi(r, \theta)=\Theta(R-r) \psi(r) \varphi_{m}(\theta)
$$

With this trial function and the flux expansion in the functional, the following is reached:

$$
\begin{aligned}
& \int_{r=0}^{r=R} r d r \int_{\theta=0}^{\theta=2 \pi} d \theta \sum_{l=0}^{\infty} D(\theta) \frac{\partial \Phi_{l}(r)}{\partial r} \frac{\partial \psi(r)}{\partial r} \varphi_{l}(\theta) \varphi_{m}(\theta) \\
& +\frac{D(\theta)}{r^{2}} \frac{\partial \varphi_{l}(\theta)}{\partial \theta} \frac{\partial \varphi_{m}(\theta)}{\partial \theta} \Phi_{l}(r) \psi(r)=\int_{r=0}^{r=R} r d r \psi(r) \int_{\theta=0}^{\theta=2 \pi} d \theta\left[S(r, \theta)-\Sigma_{t} \psi(r)\right] \varphi_{m}(\theta)
\end{aligned}
$$

The notations are simplified with: $f_{m}(r)=\int_{\theta=0}^{\theta=2 \pi} d \theta\left[S(r, \theta)-\Sigma_{t} \psi(r)\right] \varphi_{m}(\theta)$ which depends solely on the trial function and the source. The orthogonality property of the trial functions of the Sturm-Liouville operator enables further simplifications as shown below:

$$
\int_{r=0}^{r=R} r d r\left[\frac{\partial \Phi_{m}(r)}{\partial r} \frac{\partial \psi(r)}{\partial r}+\frac{\mu_{m}^{2}}{r^{2}} \Phi_{m}(r) \psi(r)\right]=\int_{r=0}^{r=R} r d r f_{m}(r) \psi(r)
$$

The first term is integrated by parts, and the flux moments $\Phi_{m}(r)$ are expressed as:

$$
\int_{r=0}^{r=R} d r\left[\frac{d}{d r}\left(r \frac{d \Phi_{m}(r)}{d r}\right)-\frac{\mu_{m}^{2}}{r} \Phi_{m}(r)+r f_{m}(r)\right] \psi(r)=0
$$

ultimately giving:

$$
\frac{d}{d r}\left(r \frac{d \Phi_{m}(r)}{d r}\right)-\frac{\mu_{m}^{2}}{r^{2}} \Phi_{m}(r)+f_{m}(r)=0
$$

Louvet solves this differential equation by expanding $f_{m}(r)$ on a polynomial basis (for which the terms tend towards 0 if a unit disc $\Omega_{0}$ is chosen):

$$
f_{m}(r)=\sum_{l=0}^{\infty} f_{m, l} r^{l}
$$

which leads to the following equation after integration and cancellation of non-finite terms at $r=0$ :

$$
\Phi_{m}(r)=\sum_{l=0}^{\infty} \frac{f_{m, l}}{\mu_{m}^{2}-(l+2)^{2}} r^{l+2}+C_{m} r^{\mu_{m}}
$$

This solution tends towards infinity at the point of the singularity when $\mu_{m}$ is less than 1. Concerning the angular part, the solution to the Sturm-Liouville problem for the media $\Omega_{1}$ and $\Omega_{2}$ are sought for under the following form:

$$
\left\{\begin{array}{l}
\varphi_{1}(\theta)=\alpha_{1}^{c} \cos (\mu \theta)+\alpha_{1}^{s} \sin (\mu \theta) \\
\varphi_{2}(\theta)=\alpha_{2}^{c} \cos (\mu \theta)+\alpha_{2}^{s} \sin (\mu \theta)
\end{array}\right.
$$

for which the continuity conditions for the angles $\theta=0$ and $\theta=\theta_{\Gamma}$ are written as:
$A:\left\{\begin{array}{l}\varphi_{1}(0)=\alpha_{1}^{c}=\varphi_{2}(2 \pi)=\alpha_{2}^{c} \cos (2 \pi \mu)+\alpha_{2}^{s} \sin (2 \pi \mu) \\ \varphi_{1}\left(\theta_{\Gamma}\right)=\alpha_{1}^{c} \cos \left(\mu \theta_{\Gamma}\right)+\alpha_{1}^{s} \sin \left(\mu \theta_{\Gamma}\right)=\alpha_{2}^{c} \cos \left(\mu \theta_{\Gamma}\right)+\alpha_{2}^{s} \sin \left(\mu \theta_{\Gamma}\right) \\ D_{1} \alpha_{1}^{s} \mu=-D_{2} \alpha_{2}^{c} \mu \sin (2 \pi \mu)+D_{2} \alpha_{2}^{s} \mu \cos (2 \pi \mu) \\ -D_{1} \alpha_{1}^{c} \mu \sin \left(\mu \theta_{\Gamma}\right)+D_{1} \alpha_{1}^{s} \mu \cos \left(\mu \theta_{\Gamma}\right)=-D_{2} \alpha_{2}^{c} \mu \sin \left(\mu \theta_{\Gamma}\right)+D_{2} \alpha_{2}^{s} \mu \cos \left(\mu \theta_{\Gamma}\right)\end{array}\right.$
The function $\varphi_{1}$ is defined only on the interval $\left[0, \theta_{\Gamma}\right]$, whereas the function $\varphi_{2}$ is defined on $\left[\theta_{\Gamma}, 2 \pi\right]$ alone. This linear system $A$ of four equations with four unknowns, $\alpha_{1}^{c}, \alpha_{1}^{s}, \alpha_{2}^{c}$ and $\alpha_{2}^{s}$, has a non-trivial solution only if its determinant is non-zero. By setting $\rho=2 \pi \mu, \gamma=\mu \theta_{\Gamma}$ and $\delta=D_{2} / D_{1}$, and by developing its determinant along the first column:

$$
\begin{aligned}
& \operatorname{det}(A)=\left|\begin{array}{cccc}
1 & 0 & -\cos \rho & -\sin \rho \\
\cos \gamma & \sin \gamma & -\cos (\gamma+\rho) & -\sin (\gamma+\rho) \\
0 & 1 & \delta \sin \rho & -\delta \cos \rho \\
-\sin \gamma & \cos \gamma & \delta \sin (\gamma+\rho) & -\delta \cos (\gamma+\rho)
\end{array}\right| \\
&=-\left(\delta^{2}+1\right) \\
& \sin \gamma \sin (\rho-\gamma)-2 \delta[1-\cos \gamma \cos (\rho-\gamma)]
\end{aligned}
$$

For the case where the angle $\theta_{\Gamma}$ is an integer multiple of $2 \pi$, such that $\theta_{\Gamma}=2 \pi / n$, this determinant is written as:

$$
\operatorname{det}_{n}(A)=-\left(\delta^{2}+1\right) \sin \gamma \sin ((n-1) \gamma)-2 \delta[1-\cos \gamma \cos ((n-1) \gamma)]
$$

Introducing Chebychev polynomials of the first kind $T_{n}(\cos \gamma)=\cos (n \lambda)$ and second kind $U_{n}(\cos \gamma)=\frac{\sin ((n+1) \lambda)}{\sin \gamma}$, the determinant is expressed under the following form (with $x=\cos \gamma$ and $y=\sin \gamma$ ):

$$
\operatorname{det}_{n}(A)=-\left(\delta^{2}+1\right) y^{2} U_{n-2}(x)-2 \delta\left[1-x T_{n-1}(x)\right]
$$

Using the recurrence relation for the Chebychev polynomials, we obtain:

$$
x T_{n-1}(x)=\frac{1}{2}\left[T_{n}(x)+T_{n-2}(x)\right]
$$

It can be seen that if $n$ is even $(n=2 k), T_{n-2}(x)$ and $T_{n}(x)$ are polynomials that have only even powers of $x$, i.e. polynomials in $x^{2}$ that can be substituted by $1-y^{2}$. Since $T_{n}(1)=1$ for any value of $n$, it can be shown that $1-x T_{n-1}(x)$ is a polynomial in $y^{2}$ without a constant term. Finally, with the polynomial expansions for $n \neq 0$ :

$$
\left\{\begin{array}{l}
T_{n}(x)=\frac{n}{2} \sum_{p=0}^{E\left(\frac{n}{2}\right)}(-1)^{p} \frac{(n-p-1)!}{p!(n-2 p)!}(2 x)^{n-2 p} \\
U_{n}(x)=\sum_{p=0}^{E\left(\frac{n}{2}\right)}(-1)^{p} \frac{(n-p)!}{p!(n-2 p)!}(2 x)^{n-2 p}
\end{array}\right.
$$

The following equation is obtained:

$$
\begin{aligned}
\operatorname{det}_{2 k}(A)= & -\left(\delta^{2}+1\right) y^{2} U_{n-2}(x) \\
& -\delta\left[2-k \sum_{p=0}^{k}(-1)^{p} \frac{(n-p-1)!}{p!(n-2 p)!} 2^{n-2 p}\left(1-y^{2}\right)^{k-p}\right. \\
& \left.-(k-1) \sum_{p=0}^{k-1}(-1)^{p} \frac{(n-p-1)!}{p!(n-2 p)!} 2^{n-2-2 p}\left(1-y^{2}\right)^{k-1-p}\right]
\end{aligned}
$$

Using the Newton binomial expansion, $x^{2 n}$ can be expanded into powers of $y^{2}$ :

$$
\left(1-y^{2}\right)^{n}=\sum_{p=0}^{n} \frac{n!}{p!(n-p)!}(-1)^{p} y^{2 p}=1+\sum_{p=1}^{n} \frac{n!}{p!(n-p)!}(-1)^{p} y^{2 p}
$$

The sum of all the coefficients of $T_{n}(x)$ and of $T_{n-2}(x)$, which is equal to 2 , can be introduced:

$$
\begin{aligned}
\operatorname{det}_{2 k}(A)= & -\left(\delta^{2}+1\right) y^{2} U_{n-2}(x) \\
+ & \delta y^{2}\left[k \sum_{p=0}^{k}(-1)^{p} \frac{(n-p-1)!}{p!(n-2 p)!} 2^{n-2 p}\left[\sum_{j=1}^{k-p} \frac{(k-p)!}{j!(k-p-j)!}(-1)^{j} y^{2 j-2}\right]\right] \\
+ & \delta y^{2}\left[(k-1) \sum_{p=0}^{k-1}(-1)^{p} \frac{(n-p-1)!}{p!(n-2 p)!} 2^{n-2-2 p}\left[\sum_{j=1}^{k-1-p} \frac{(k-1-p)!}{j!(k-1-p-j)!}(-1)^{j} y^{2 j-2}\right]\right] \\
& =y^{2}\left(-\left(\delta^{2}+1\right) U_{n-2}(x)+\delta V_{k}\left(y^{2}\right)\right)
\end{aligned}
$$

The goal of this demanding calculation is to show that the determinant cancels out in two cases:

$$
\left\{\begin{array}{l}
y^{2}=0 \\
-\left(\delta^{2}+1\right) \quad U_{n-2}(x)+\delta V_{k}\left(y^{2}\right)=0
\end{array}\right.
$$

The first equation highlights the fact that $y^{2}=\sin ^{2}\left(\mu \theta_{\Gamma}\right)=0$, i.e. $\mu \theta_{\Gamma}=\mu \frac{2 \pi}{2 k}=m \pi$. The second is a transcendental equation in $\mu \theta_{\Gamma}$ that will be discussed only for the case where $n=4$, i.e. where $\theta_{\Gamma}$ is a right angle. The latter case is especially interesting for the inward and outward corners of a $P W R$ core.

$$
\begin{aligned}
\operatorname{det}_{4}(A) & =-\left(\delta^{2}+1\right) \sin \gamma \sin (3 \gamma)-2 \delta[1-\cos \gamma \cos (3 \gamma)] \\
& =-\left(\delta^{2}+1\right) \sin ^{2} \gamma(1+2 \cos (2 \gamma)) \\
& -2 \delta\left[\sin ^{2} \gamma+\cos ^{2} \gamma-\left(\cos (2 \gamma) \cos ^{2} \gamma-2 \sin ^{2} \gamma \cos ^{2} \gamma\right)\right] \\
& =-\sin ^{2} \gamma\left[\left(2 \delta^{2}+4 \delta+2\right) \cos (2 \gamma)+\delta^{2}+6 \delta+1\right]
\end{aligned}
$$

The determinant becomes zero for two sets of eigenvalues:

$$
\gamma=\mu_{m} \frac{\pi}{2}=m \pi \quad m \geq 1 \quad \text { or } 2 \gamma=\mu_{m} \pi=\arccos \frac{-\left(\delta^{2}+6 \delta+1\right)}{\left(2 \delta^{2}+4 \delta+2\right)}+2 m \pi \quad m \geq 0
$$

The function $f_{4}(\delta)=\frac{-\left(\delta^{2}+6 \delta+1\right)}{\left(2 \delta^{2}+4 \delta+2\right)}$ that appears in the inverse-cosine is always contained in the interval $\left[-1,-\frac{1}{2}\right]$ with a minimum value that occurs for $f$ $(\delta=1)=-1$, corresponding to the homogeneous case when both media have the same diffusion coefficient, and there is no singularity since $\mu_{m}=1$. The conditions $\mu_{m} \geq 1$ or $\mu_{m}=0$ are required to obtain a regular flux $\Phi(r, \theta)$ at the singularity for $\delta \neq 1$. The first condition is always verified although this is not always the case for the second condition. Indeed, analysis of the function $f_{4}(\delta)$ shows that:

$$
\frac{2}{3} \leq \mu_{m}=\frac{1}{\pi} \arccos \frac{-\left(\delta^{2}+6 \delta+1\right)}{\left(2 \delta^{2}+4 \delta+2\right)} \leq 1
$$

Thus this first mode represents the flux singularity at the origin. For odd values of $n$ (this is the case for hexagons in fast reactor lattices where the angle between the faces is equal to $2 \pi / 3$ ), the roots of the discriminant are solutions of a transcendental equation that cannot be factorized in a simple term, and has to be evaluated for each case. To deal with problems at the boundaries of the reactor where the flux is assumed to be zero on the perimeter of the corner, the latter being such that one of its die coincides with the $2 \pi$ direction by rotational symmetry of the figure, the boundary conditions lead to:

$$
B:\left\{\begin{array}{l}
\varphi_{1}(2 \pi)=\alpha_{2}^{c} \cos \left(2 \pi \mu_{m}\right)+\alpha_{2}^{s} \sin \left(2 \pi \mu_{m}\right)=0 \\
\varphi_{1}\left(\theta_{\Gamma}\right)=\alpha_{1}^{c} \cos \left(\mu_{m} \theta_{\Gamma}\right)+\alpha_{1}^{s} \sin \left(\mu_{m} \theta_{\Gamma}\right)=0
\end{array}\right.
$$

This system has a non-trivial solution if:

$$
\mu_{m}=\frac{m \pi}{\theta_{\Gamma}}
$$

The flux, then, has a singularity if $\theta_{\Gamma}>\pi$, which is the case of inward corners on the perimeter of a $P W R\left(\theta_{\Gamma}=3 \pi / 2\right)$.
D.G. Cacuci generalized this approach ${ }^{13}$ in multi-group theory to deal with multi-corners forming singularities between several domains having constant properties (Fig. 12.13). In his approach, he develops the flux in the following form:

$$
\Phi_{g}(r, \theta)=\sum_{l=0}^{\infty} \Phi_{l, g}(r) \varphi_{l, g}(\theta)
$$

where $g$ is the index for the energy group in a multi-group approach and $\varphi_{l, g}(\theta)$, with a $2 \pi$ period, are the eigenfunctions of the groupwise Sturm-Liouville equation with continuous angular pseudo-current and the continuity of $\varphi_{l, g}\left(\theta_{n}\right)$ (Picture 12.3).

The functions $\varphi_{l, g}(\theta)$ satisfy the orthogonality relation:

[^269]Picture 12.3 Dan Cacuci (Courtesy Cacuci)


Fig. 12.13 Multi-corner for a domain in two dimensions


$$
\left\{\begin{array}{l}
\int_{0}^{2 \pi} D_{g}(\theta) \varphi_{n, g}(\theta) \varphi_{m, g}(\theta) d \theta=N_{m, g} \delta_{n, m} \\
\int_{0}^{2 \pi} D_{g}(\theta) \frac{d \varphi_{n, g}(\theta)}{d \theta} \frac{d \varphi_{m, g}(\theta)}{d \theta} d \theta=\mu_{m, g}^{2} N_{m, g} \delta_{n, m}
\end{array}\right.
$$

where $N_{m, g}$ is the normalization coefficient that depends on the geometry. The introduction of such a flux expansion in the multi-group diffusion equation:

$$
\begin{aligned}
& -\operatorname{div}\left(D_{g}(\theta) \overrightarrow{\operatorname{grad}} \Phi_{g}(r, \theta)\right) \Phi_{g}(r, \theta)+\Sigma_{t}(\theta) \Phi_{g}(r, \theta) \\
& =\sum_{g^{\prime}=1}^{G} \Sigma_{s}^{g^{\prime} \rightarrow g}(\theta) \Phi_{g^{\prime}}(r, \theta)+\chi_{g^{\prime}} \frac{\nu \Sigma_{f, g^{\prime}}(\theta) \Phi_{g^{\prime}}(r, \theta)}{k_{e f f}}
\end{aligned}
$$

leads to a differential equation on the flux moments $\Phi_{l, g}(r)$ similar to that obtained for a unique angle, but containing a coupling term for the energy groups. Cacuci applied this formulation to the corners of the hexagons in the lattice of a fast reactor and showed that the multi-group flux was continuous at the singularity, but that it cannot be expressed analytically. In particular, the derivative of the spatial flux is not continuous, thereby invalidating the expansion into Taylor series at the singularity. However, Louvet's numerical studies showed that for $P W R$, the singularities deteriorated the order of convergence slightly for the spatial flux in a core calculation, especially for nodal methods. Hence, it is inadvisable to employ singular functions to represent flux behavior locally, close to singularities, since this operation is both complex and time-consuming.

### 12.5.10 Anisotropic Point Source in a Multiplying Medium

The case of a point source in a non-multiplying medium was illustrated earlier in the chapter "The diffusion approximation in neutronics". The condition of:

$$
\frac{k_{\infty}-1}{M^{2}}<0
$$

comes from similar calculations. However, if $B_{m}^{2} \equiv\left(k_{\infty}-1\right) / M^{2}>0$, the calculations are slightly different.

The diffusion equation with a point source is written as:

$$
\Delta \Phi(r, \theta, \varphi)+\frac{k_{\infty}-1}{M^{2}} \Phi(r, \theta, \varphi)=S\left(x_{0}, y_{0}, z_{0}\right)
$$

Using the hypothesis of separation of variables, $\Phi(r, \theta, \varphi) \equiv f(\cos \theta) g(\varphi) h(r)$, this leads to a slightly different system of differential equations:

$$
\left\{\begin{array}{l}
\sin ^{2} \theta \frac{d^{2} f}{d(\cos \theta)^{2}}+2 \cos \theta \frac{d f}{d(\cos \theta)}+\left(n(n+1)-\frac{m^{2}}{\sin ^{2} \theta}\right) f=0 \\
\frac{d^{2} g}{d \varphi^{2}}+m^{2} g=0 \\
\frac{d^{2} h}{d r^{2}}+\frac{2 d h}{r d r}+\left(B_{m}^{2}-\frac{n(n+1)}{r^{2}}\right) h=0
\end{array}\right.
$$

The equation in $r$ is a non-modified spherical Bessel equation of the form (Abramowitz and Stegun 1972, p. 437):

$$
\rho^{2} \frac{d^{2} h}{d \rho^{2}}+2 \rho \frac{d h}{d \rho}+\left(\rho^{2}-n(n+1)\right) h=0 \text { where } \rho \equiv B_{m} r
$$

and for which the solution that decays at infinity is a Hankel function of the second kind:

$$
h_{n}^{(2)}(\rho)=\sqrt{\frac{1}{2} \frac{\pi}{\rho}} H_{n+\frac{1}{2}}(\rho)
$$

Since $H_{\nu}(\rho)=\sqrt{\frac{2}{\pi \rho}} e^{-i\left(\rho-\frac{1}{2} \nu \pi-\frac{1}{4}\right)}, h_{0}^{(2)}(\rho)=\sqrt{\frac{1}{2} \frac{\pi}{\rho}} H_{\frac{1}{2}}(\rho)=\frac{1}{\rho} e^{-i\left(\rho-\frac{\pi}{2}\right)}=\frac{i}{\rho} e^{-i \rho}$ can be computed.

With the same methodology as that illustrated in diffusion, by taking the limit, the following expression is determined:

$$
\lim _{a \rightarrow 0}<S, \Phi>=\int_{\theta=0}^{\theta=\pi} \sin \theta d \theta \int_{\varphi=0}^{\varphi=2 \pi} d \varphi\left(-\frac{i}{B_{m}} \Phi\left(x_{0}, y_{0}, z_{0}\right)\right)=-\frac{4 \pi i}{B_{m}} \Phi\left(x_{0}, y_{0}, z_{0}\right)
$$

Thus, the source corresponding to the function $\psi_{0}^{0}(r)=\frac{i}{\rho} e^{-i \rho}$ is given by $S_{0}^{0}=-\frac{4 \pi i}{B_{m}} \delta\left(x-x_{0}, y-y_{0}, z-z_{0}\right)$. These conclusions in a multiplying medium are the same as in the case of diffusion in a non-multiplying medium.

### 12.5.11 Zero Flux Distance

In the previous cases, for simplification, flux was assumed to be zero at the limit of the objects under consideration (e.g. at radius $R$ for a sphere). In the case of actual reactors, the flux (or rather its prolongation in the mathematical sense) cancels outside the volume corresponding to the reactor at the distance where the flux becomes zero. This distance corresponds to the position where the flux of a bare reactor in fundamental mode would be zero (this definition differs from the extrapolation distance, which will be discussed later). Hence, the flux is non-zero at the reactor limits due to the presence of a medium surrounding the core, called the reflector, the purpose of which is to reflect neutrons back into the core, as will be seen below. The results for the flux shape are absolutely identical if, in the case of the sphere, the radius $R$ is substituted by $R+\delta$ (or $H$ by $H+\delta$ for the cylinder) in the equations. For large reactors, $\delta$ is usually negligible compared to the size of the reactor. In the case illustrated here, only a cylindrical finite reactor, which is very
similar to a $P W R$, is considered. The flux shape in a cylindrical reactor is expressed as:

$$
\Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R} r\right) \cos \left(\frac{\pi}{H} z\right) .
$$

The zero-flux distance for a $P W R$ is of the order of $\delta \approx 40 \mathrm{~cm}$. To simplify, it can be assumed that the flux is zero at the same distance from the active core in both the radial and axial directions (whereas in a real reactor, the properties of the radial and axial reflectors are different). The flux shape is thus given by $\Phi_{\max } J_{0}\left(j_{0,1} r /(R+\delta)\right)$ $\cos (\pi z /(H+2 \delta))$. The mean flux, usually used to compute the core power, is given by:

$$
\bar{\Phi}=\frac{\int_{r=0}^{r=R} \int_{\theta=0}^{\theta=2 \pi} \int_{z=-\frac{H}{2}}^{z=+\frac{H}{2}} \Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R+\delta} r\right) \cos \left(\frac{\pi}{H+2 \delta} z\right) d z r d \theta d r}{\pi R^{2} H}
$$

Hence:

$$
\begin{aligned}
\frac{\bar{\Phi}}{\Phi_{\max }} & =\frac{\frac{H+2 \delta}{\pi}\left[\sin \left(\frac{\pi}{H+2 \delta} z\right)\right]_{z=-\frac{H}{2}}^{z=+\frac{H}{2}} 2 \pi \int_{r=0}^{r=R} J_{0}\left(\frac{j_{0,1}}{R+\delta} r\right) r d r}{\pi R^{2} H} \\
= & \frac{4 \frac{H+2 \delta}{\pi} \sin \left(\frac{\pi}{H+2 \delta} \frac{H}{2}\right) \frac{R+\delta}{j_{0,1}} J_{1}\left(\frac{j_{0,1}}{R+\delta} R\right)}{R H}
\end{aligned}
$$

Assuming that $\delta \ll H$ and that $\delta \ll R$, the previous formula can be expanded using a Taylor series such that:

$$
J_{1}\left(\frac{j_{0,1}}{R+\delta} R\right) \approx J_{1}\left(j_{0,1}\left(1-\frac{\delta}{R}\right)\right)=J_{1}\left(j_{0,1}\right)-j_{0,1} \frac{\delta}{R} J_{1}^{\prime}\left(j_{0,1}\right)+\ldots
$$

Using the recurrence relation: $x J_{n}^{\prime}(x)=-n J_{n}(x)+x J_{n-1}(x)$, we obtain:

$$
j_{0,1} J_{1}^{\prime}\left(j_{0,1}\right)=-J_{1}\left(j_{0,1}\right)+j_{0,1} \underbrace{J_{0}\left(j_{0,1}\right)}_{0}=-J_{1}\left(j_{0,1}\right)
$$

Hence: $\quad J_{1}\left(\frac{j_{0,1}}{R+\delta} R\right) \approx J_{1}\left(j_{0,1}\right)+\frac{\delta}{R} J_{1}\left(j_{0,1}\right)+\ldots$
Since: $\quad \sin \left(\frac{\pi H}{H+2 \delta 2}\right) \approx \sin \left(\frac{\pi}{2}\left(1-\frac{2 \delta}{H}\right)\right)=\cos \left(\frac{2 \delta}{H}\right) \approx 1-\frac{2 \delta^{2}}{H^{2}}$.
By substituting in the flux expression, the following equation is obtained:

$$
\begin{gathered}
\bar{\Phi}=\frac{4 H \frac{1+\frac{2 \delta}{H}}{\pi}\left(1-\frac{2 \delta^{2}}{H^{2}}\right)}{} R \frac{1+\frac{\delta}{R}}{j_{0,1}}\left(J_{1}\left(j_{0,1}\right)+\frac{\delta}{R} J_{1}\left(j_{0,1}\right)\right) \\
R H \\
\bar{\Phi}=\left(\frac{4}{\pi j_{0,1}} J_{1}\left(j_{0,1}\right)+\frac{8}{\pi j_{0,1}}\left(\frac{1}{H}+\frac{1}{R}\right) J_{1}\left(j_{0,1}\right) \delta+\frac{4}{\pi j_{0,1}}\left(\frac{4}{H R}+\frac{1}{R^{2}}-\frac{2}{H^{2}}\right) \delta^{2}+O\left(\delta^{3}\right)\right) \Phi_{\max }
\end{gathered}
$$

At order 0 in $\delta$, the following equation $\bar{\Phi}=4 J_{1}\left(j_{0,1}\right) \quad \Phi_{\max } /\left(\pi j_{0,1}\right)$ is obtained for a cylindrical reactor with null flux boundary conditions. The previous calculation gives the first-order term in $\delta$ and is useful for analyzing the effect of a possible reflector around the core on flattening of the flux, a condition sought to optimize fuel use-up and limit power peaks.

### 12.5.12 Annular Reactor

(Etherington 1957, pp. 6-67).
The geometry of a reactor can be made more complex depending on the applications. However, the criticality condition cannot always be expressed in terms of a simple formula as:

$$
B_{g}^{2}=\frac{k_{\infty}-1}{M^{2}}
$$

which has the didactic interest of separating geometrical dependences (geometrical buckling) from material properties (material buckling), since the geometrical buckling of a reactor cannot always be simply obtained. The example of the annular reactor (Fig. 12.14) illustrates this problem very well.

The one-energy group diffusion equation in a homogeneous multiplying medium without any further source is expressed as follows using the usual conventions and simplified using the material buckling:

$$
-D \Delta \Phi+\Sigma_{a} \Phi=\nu \Sigma_{f} \Phi \text { thus, } \Delta \Phi-\frac{\Sigma_{a}}{D} \Phi+\frac{\nu \Sigma_{f}}{D} \Phi=0
$$

Hence: $\quad \Delta \Phi+B_{m}^{2} \Phi=0$ with $B_{m}^{2}=\frac{k_{\infty}-1}{M^{2}}, M^{2}=\frac{D}{\Sigma_{a}}$ and $k_{\infty}=\frac{\nu \Sigma_{f}}{\Sigma_{a}}$
The flux shape can be computed in terms of the radius and maximum flux of the reactor, assuming that the cylinder is infinite in the $z$ direction, and assuming that the flux is zero at the reactor boundaries. The flux solution is written as:

$$
\Phi(r)=a J_{0}\left(B_{m} r\right)+b Y_{0}\left(B_{m} r\right)
$$

Constants $a$ and $b$ are determined using the boundary conditions:

Fig. 12.14 Critical
cylindrical annular reactor of inner radius $R_{i}$ and outer radius $R_{e}$


$$
\left\{\begin{array}{c}
\Phi\left(R_{i}\right)=a J_{0}\left(B_{m} R_{i}\right)+b \quad Y_{0}\left(B_{m} R_{i}\right)=0 \\
\Phi\left(R_{e}\right)=a J_{0}\left(B_{m} R_{e}\right)+b \quad Y_{0}\left(B_{m} R_{e}\right)=0
\end{array}\right.
$$

This linear system leads to a trivial solution $a=0$ and $b=0$, except in the case where the two equations are related, i.e.

Criticality condition for the annular reactor:

$$
\left|\begin{array}{ll}
J_{0}\left(B_{m} R_{i}\right) & Y_{0}\left(B_{m} R_{i}\right)  \tag{12.14}\\
J_{0}\left(B_{m} R_{e}\right) & Y_{0}\left(B_{m} R_{e}\right)
\end{array}\right|=J_{0}\left(B_{m} R_{i}\right) \quad Y_{0}\left(B_{m} R_{e}\right)-J_{0}\left(B_{m} R_{e}\right) \quad Y_{0}\left(B_{m} R_{i}\right)=0
$$

This equation, which relates the geometrical data to material data, is the criticality condition. In this example, the criticality condition is a transcendental equation that relates the geometry (with $R_{i}$ and $R_{e}$ of the reactor) and material properties (material buckling $B_{m}$ ). In the fundamental mode of this reactor, the flux is zero at its inner and outer boundaries and may be assumed to be maximal at radius $R_{\text {max }}$ :

$$
\Phi\left(R_{\max }\right)=a J_{0}\left(B_{m} R_{\max }\right)+b Y_{0}\left(B_{m} R_{\max }\right)=\Phi_{\max }
$$

In addition, the flux derivative is zero at $R_{\max }$ :

$$
\frac{\partial \Phi}{\partial r}\left(R_{\max }\right)=-a B_{m} J_{1}\left(B_{m} R_{\max }\right)-b B_{m} Y_{1}\left(B_{m} R_{\max }\right)=0
$$

With these two equations, coefficients $a$ and $b$ are expressed in terms of $\Phi_{\text {max }}$ and $R_{\text {max }}$ :

$$
\left\{\begin{array}{l}
a=\frac{\left|\begin{array}{cc}
\Phi_{\max } & Y_{0}\left(B_{m} R_{\max }\right) \\
0 & B_{m} Y_{1}\left(B_{m} R_{\max }\right)
\end{array}\right|}{\left|\begin{array}{cc}
J_{0}\left(B_{m} R_{\max }\right) & Y_{0}\left(B_{m} R_{\max }\right) \\
B_{m} J_{1}\left(B_{m} R_{\max }\right) & B_{m} Y_{1}\left(B_{m} R_{\max }\right.
\end{array}\right|}=\frac{\Phi_{\max } Y_{1}\left(B_{m} R_{\max }\right)}{J_{0}\left(B_{m} R_{\max }\right) Y_{1}\left(B_{m} R_{\max }\right)-J_{1}\left(B_{m} R_{\max }\right) Y_{0}\left(B_{m} R_{\max }\right)} \\
b=\frac{\left|\begin{array}{cc}
J_{0}\left(B_{m} R_{\max }\right) & \Phi_{\max } \\
B_{m} J_{1}\left(B_{m} R_{\max }\right) & 0
\end{array}\right|}{\left|\begin{array}{cc}
J_{0}\left(B_{m} R_{\max }\right. & Y_{0}\left(B_{m} R_{\max }\right) \\
B_{m} J_{1}\left(B_{m} R_{\max }\right) & B_{m} Y_{1}\left(B_{m} R_{\max }\right)
\end{array}\right|}=\frac{-\Phi_{\max } J_{1}\left(B_{m} R_{\max }\right)}{J_{0}\left(B_{m} R_{\max }\right) Y_{1}\left(B_{m} R_{\max }\right)-J_{1}\left(B_{m} R_{\max }\right) Y_{0}\left(B_{m} R_{\max }\right)}
\end{array}\right.
$$

Furthermore, it can be seen that, with the boundary conditions, the ratio $a / b$ is worth:

$$
\frac{a}{b}=-\frac{Y_{1}\left(B_{m} R_{\max }\right)}{J_{1}\left(B_{m} R_{\max }\right)}=-\frac{Y_{0}\left(B_{m} R_{i}\right)}{J_{0}\left(B_{m} R_{i}\right)}=-\frac{Y_{0}\left(B_{m} R_{e}\right)}{J_{0}\left(B_{m} R_{e}\right)}
$$

Thus, another transcendental equation is reached that allows the calculation of $R_{\text {max }}$ in terms of either $B_{m} R_{i}$, or $B_{m} R_{e}$, which are both equivalent thanks to the criticality condition. Therefore, an approximation of the radius for which the maximum flux is reached may be expressed in terms of the geometrical data and the material buckling, assuming a "weakly annular reactor", i.e. $\delta_{i}=R_{\max }-R_{i} \ll R_{i}$. Hence, the Bessel functions can be expanded into a Taylor series at order 1:

$$
\frac{Y_{1}\left(B_{m} R_{\max }\right)}{J_{1}\left(B_{m} R_{\max }\right)}=\frac{Y_{1}\left(B_{m}\left(R_{i}+\delta_{i}\right)\right)}{J_{1}\left(B_{m}\left(R_{i}+\delta_{i}\right)\right)} \approx \frac{Y_{1}\left(B_{m} R_{i}\right)+B_{m} \delta_{i} Y_{1}^{\prime}\left(B_{m} R_{i}\right)}{J_{1}\left(B_{m} R_{i}\right)+B_{m} \delta_{i} J_{1}^{\prime}\left(B_{m} R_{i}\right)}
$$

Equating the two expressions for the ratio $a / b$ leads to:

$$
\begin{aligned}
& \frac{Y_{1}\left(B_{m} R_{i}\right)+B_{m} \delta_{i} Y_{1}^{\prime}\left(B_{m} R_{i}\right)}{J_{1}\left(B_{m} R_{i}\right)+B_{m} \delta_{i} J_{1}^{\prime}\left(B_{m} R_{i}\right)}=\frac{Y_{0}\left(B_{m} R_{i}\right)}{J_{0}\left(B_{m} R_{i}\right)} \\
& \text { thus: } \quad \delta_{i}=\frac{J_{1}\left(B_{m} R_{i}\right) Y_{0}\left(B_{m} R_{i}\right)-Y_{1}\left(B_{m} R_{i}\right) J_{0}\left(B_{m} R_{i}\right)}{B_{m} Y_{1}^{\prime}\left(B_{m} R_{i}\right) J_{0}\left(B_{m} R_{i}\right)-B_{c} J_{1}^{\prime}\left(B_{m} R_{i}\right) Y_{0}\left(B_{m} R_{i}\right)}
\end{aligned}
$$

It can be proven that if the inner radius $R_{i}$ tends towards $0, \delta_{i}$ also tends towards 0 . To simplify the notations, let $x=B_{m} R_{i}$. The derivatives of the Bessel functions are calculated using the recurrence relations:

$$
\left\{\begin{aligned}
Y_{1}^{\prime}(x) & =-\frac{1}{x} Y_{1}(x)+Y_{0}(x) \\
J_{1}^{\prime}(x) & =-\frac{1}{x} J_{1}(x)+J_{0}(x)
\end{aligned}\right.
$$

In the neighborhood of 0, the Taylor series of the first Bessel functions are:

$$
\begin{cases}J_{0}(x) \approx 1-\frac{x^{2}}{4} & Y_{0}(x) \approx \frac{2}{\pi}\left[\ln \left(\frac{x}{2}\right) J_{0}(x)\right] \approx \frac{2}{\pi} \ln (x) \\ J_{1}(x) \approx \frac{x}{2}\left(1-\frac{x^{2}}{8}\right) & Y_{1}(x) \approx-\frac{1}{\pi} \Gamma(1) \frac{1}{\left(\frac{1}{2} x\right)}=-\frac{2}{\pi x}\end{cases}
$$

The value of $\delta_{i}$ is approximated by:

$$
\begin{aligned}
& \delta_{i} \approx \frac{\frac{x}{2}\left(1-\frac{x^{2}}{8}\right)\left(\frac{2}{\pi} \ln (x)\right)-\left(-\frac{2}{\pi x}\right)\left(1-\frac{x^{2}}{4}\right)}{B_{m}\left(-\frac{1}{x} Y_{1}(x)+Y_{0}(x)\right)\left(1-\frac{x^{2}}{4}\right)-B_{m}\left(-\frac{1}{x} J_{1}(x)+J_{0}(x)\right) \frac{2}{\pi} \ln (x)} \\
& \text { Hence: } \lim _{x \rightarrow 0}\left(\delta_{i}\right)=\lim _{x \rightarrow 0}\left(\frac{\frac{x^{3}}{2} \frac{2}{\pi} \ln (x)+\frac{2}{\pi} x}{B_{m}\left(\frac{2}{\pi}\right)}\right)=\lim _{x \rightarrow 0}\left(\frac{x}{B_{m}}\right)
\end{aligned}
$$

Therefore, $\delta_{i}=R_{\max }-R_{i}$ tends towards 0 when $x$ tends towards 0 , which is intuitive since this case tends towards the infinite cylindrical reactor where the flux is maximum at its center (except for the boundary condition on the inner radius). Similarly, it can be shown that $\delta_{e}=R_{e}-R_{\max }$ tends towards $R_{e}$. The maximum flux is determined with the desired power level of the reactor (with the mean flux obtained via an integration on the reactor). This textbook case illustrates that the criticality condition can be expressed for complex geometries (an industrial reactor) by cancelling the determinant of the linear system of boundary conditions (equivalent to seeking a non-trivial solution for which the flux has a non-zero value). These conditions will couple the geometrical data of the reactor to the neutronic properties of its constituent materials. On the other hand, this case also shows that the flux is known up to a constant (either the maximum flux or the mean flux) since the diffusion equation has an infinite number of co-linear solutions. In the case where a non-zero flux at the boundaries is required for instance, we have:

$$
\left\{\begin{array}{cc}
\Phi\left(R_{i}\right)=a & J_{0}\left(B_{m} R_{i}\right)+b \quad Y_{0}\left(B_{m} R_{i}\right)=\Phi_{i} \\
\Phi\left(R_{e}\right)=a & J_{0}\left(B_{m} R_{e}\right)+b \quad Y_{0}\left(B_{m} R_{e}\right)=\Phi_{e}
\end{array}\right.
$$

The solution to the linear system entails the fact that the coefficients $a$ and $b$ depend on the boundary conditions, on the geometry via $R_{i}$ and $R_{e}$, and on $B_{m}$ $=\sqrt{\left(k_{\infty} / k_{\text {eff }}-1\right) / M^{2}}$ by re-injecting the $k_{\text {eff }}$ of the theoretical critical reactor. This $k_{\text {eff }}$ value depends on the addition of a closure relation, according to a principle discussed in the slab case. For instance, this equation can be the maximum flux value at a radius $R_{\text {max }}$ or the mean flux value on the whole reactor, or the current $J=-D \operatorname{grad} \Phi$, either at $R_{i}$ or at $R_{e}$ (but not both at the same time!). Each of these choices leads to a different value of $k_{\text {eff }}$.

### 12.6 Any Three-Dimensional Reactor

In the general case, there is no analytical solution and only use of a computer enables solution of the problem using iterative methods. The $2 D-1 D$ fusion method, also called the alternate iterative flux method, is a way to reconstruct the $3 D$ information. The method consists in calculating the flux in a given direction (axial one for e.g.) with a radial leakage coefficient, and each $2 D$ layer is then computed using the leakage at the previous step, with the iteration continuing until convergence. It is adapted for a reactor that has a strong radial heterogeneity, but not axially, as for a $P W R$. The discretized diffusion equation according to the geometrical blocks in Cartesian geometry, is written as follows, after integration over the blocks.:

$$
\begin{aligned}
& -D \int_{\Delta x} \int_{\Delta y} d x d y \int_{\Delta z} \frac{\partial^{2} \Phi}{\partial z^{2}}-D \int_{\Delta z} d z \int_{\Delta x} \int_{\Delta y}\left(\frac{\partial^{2} \Phi}{\partial x^{2}}+\frac{\partial^{2} \Phi}{\partial y^{2}}\right) d x d y \\
& +\Sigma_{a} \int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \Phi d x d y d z=\frac{\int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \nu \Sigma_{f} \Phi d x d y d z}{k_{e f f}}
\end{aligned}
$$

The following equations are used to simplify the notations, and the local geometrical buckling terms are introduced ${ }^{14}$ :

$$
\begin{aligned}
& \Phi_{z}=\int_{\Delta x} \int_{\Delta y} \Phi d x d y, \quad \Phi_{x y}=\int_{\Delta z} \Phi d z, F_{x y}=\frac{\int_{\Delta z} \nu \Sigma_{f} \Phi d z}{k_{e f f}}, F_{z}=\frac{\int_{\Delta x} \int_{\Delta y} \nu \Sigma_{f} \Phi d z}{k_{e f f}} \\
& B_{z}^{2}=-D \frac{\int_{\Delta x} \int_{\Delta y} d x d y \int_{\Delta z} \frac{\partial^{2} \Phi}{\partial z^{2}}}{\int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \Phi d x d y d z}, \quad B_{x y}^{2}=-D \frac{\int_{\Delta z} d z \int_{\Delta x} \int_{\Delta y}\left(\frac{\partial^{2} \Phi}{\partial x^{2}}+\frac{\partial^{2} \Phi}{\partial y^{2}}\right) d x d y}{\int_{\Delta x} \int_{\Delta y} \int_{\Delta z} \Phi d x d y d z}
\end{aligned}
$$

The $3 D$ equation is expressed as two equations with alternate directions:

$$
\left\{\begin{array}{c}
-D \int_{\Delta x} \int_{\Delta y} d x d y \int_{\Delta z} \frac{\partial^{2} \Phi_{z}}{\partial z^{2}}+\int_{\Delta z}\left(\Sigma_{a}+D B_{x y}^{2}\right) \Phi_{z} d z=\int_{\Delta z} F_{z} d z \\
-D \int_{\Delta x} \int_{\Delta y}\left(\frac{\partial^{2} \Phi_{x y}}{\partial x^{2}}+\frac{\partial^{2} \Phi_{x y}}{\partial y^{2}}\right) d x d y+\int_{\Delta x} \int_{\Delta y}\left(\Sigma_{a}+B_{z}^{2}\right) \Phi_{x y} d x d y d z=\int_{\Delta x} \int_{\Delta y} F_{x y} d x d y
\end{array}\right.
$$

where $\Phi_{z}$ and $\Phi_{x y}$ are 1D and 2D solutions of the diffusion equation:

[^270]\[

\left\{$$
\begin{array}{c}
-D \frac{\partial^{2} \Phi_{z}}{\partial z^{2}}+\left(\Sigma_{a}-D \frac{\int_{\Delta x} \int_{\Delta y}\left(\frac{\partial^{2} \Phi_{x y}}{\partial x^{2}}+\frac{\partial^{2} \Phi_{x y}}{\partial y^{2}}\right) d x d y}{\int_{\Delta x} \int_{\Delta y} \Phi_{x y} d z}\right) \Phi_{z}=F_{z} \\
-D\left(\frac{\partial^{2} \Phi_{x y}}{\partial x^{2}}+\frac{\partial^{2} \Phi_{x y}}{\partial y^{2}}\right)+\left(\Sigma_{a}-\frac{\int_{\Delta z} \frac{\partial^{2} \Phi_{z}}{\partial z^{2}}}{\int_{\Delta z} \Phi_{z} d z}\right) \Phi_{x y}=F_{x y}
\end{array}
$$\right.
\]

The convergence criterion for the flux is obtained when:

$$
\left|\frac{\int_{\Delta z} \Phi_{z} d z-\int_{\Delta x} \int_{\Delta y}\left(\frac{\partial^{2} \Phi_{x y}}{\partial x^{2}}+\frac{\partial^{2} \Phi_{x y}}{\partial y^{2}}\right) d x d y}{\int_{\Delta z} \Phi_{z} d z}\right| \leq \varepsilon
$$

When fluxes $\Phi_{z}$ and $\Phi_{x y}$ are converged, the source terms $F_{z}$ and $F_{x y}$ are computed over again, and iterations are carried out over these sources until they converge (power iteration method). The $2 D$ calculations themselves can be broken down into two $l D$ calculations, with more or less acceptable results [transverse leakage method, (Walter and Reynolds 1981, p. 107)], except for some geometries such that of a lattice of fissile slabs (e.g. submarine reactors).

For more general cases in which sufficient computational power is available, the reactor can be modeled in three dimensions, for instance in France in the case of the COCCINELLE code at EDF or CRONOS2 for CEA. The critical system set-up includes all the cells of the calculation mesh that are coupled through the interface conditions. These matrices are massively empty since each cell usually has few interfaces ( 6 in the case of a parallelepiped). A wise choice of numbering for the nodes leads to a matrix that is conditioned in an efficient manner, for instance, with hexagonal assemblies, where along some edges a regular mesh is obtained. Since most numerical methods are sensitive to matrix conditioning methods, this particular aspect must be studied carefully to avoid degrading the computational times.

### 12.7 Fermi Age Theory

(Bonilla 1957, p. 193; Etherington 1957, pp. 6-45; Ferziger and Zweifel 1966, p. 146; Meghreblian and Holmes 1960, p. 268).

Fermi's age theory was developed by Enrico Fermi at a time when the variation of cross sections with energy was not well known, and the first computers were not powerful enough for multi-group calculations. The significant development of scientific computing and the present knowledge of basic nuclear data have rendered this method obsolete. Nevertheless, it is still useful to understand the physics of the energy phenomena occurring inside a reactor.

### 12.7.1 History

In 1942, Fermi built a critical pile (literally a pile of graphite) under the stands of the Chicago stadium. The moderator was very pure and weakly absorbing graphite, for which the mean lethargy gain per collision is small. He substituted the discontinuous slowing-down process-through collisions on carbon atoms of atomic mass $12(\xi=0.158)$-by a continuous process. This approach allowed him to theoretically compute the neutron spectrum in the pile (Fig. 12.15 and Picture 12.4).


Fig. 12.15 A sketch of Fermi's pile autographed by its conceivers. Only one picture remains of the graphite blocks and the pile itself. (Public domain)

## Picture 12.4 Enrico

Fermi, Physics Nobel Prize
winner in 1938 (Public
domain)


His mathematical formalism included a quantity that is dimensionally homogeneous to a surface area, called the Fermi age $\tau$. It is particularly valid for graphite but can be extended, under some conditions, to other moderators such as water.

### 12.7.2 Overview of Slowing-Down

In Chap. 4 on slowing-down, we found out that the mean lethargy gain per collision is:

Mean lethargy gain: $\xi=\overline{\Delta u}=\int_{0}^{\log (1 / \alpha)} v P(v) d v=\int_{\alpha E_{0}}^{E_{0}} \ln \left(\frac{E_{0}}{E}\right) P(E) d E$

$$
\begin{equation*}
=1+\frac{\alpha}{1-\alpha} \ln (\alpha) \tag{12.15}
\end{equation*}
$$

In Fermi's pile (a critical pile moderated by graphite, thus carbon), where energy loss is weak (i.e. $\Delta E \ll E_{0}, E_{0}$ being the energy at which collision occurs), we obtain:

$$
\overline{\Delta u}=\overline{\ln \left(E_{0}\right)-\ln \left(E_{0}-\Delta E\right)} \quad \Rightarrow \xi \approx \overline{\ln \left(1+\frac{\Delta E}{E_{0}}\right)} \quad \Rightarrow \xi \approx \frac{\overline{\Delta E}}{E_{0}}
$$

If the phenomenon is continuous, it can be assumed that this expression can be extended to a derivative: $\xi=d E / E$. Let $\lambda_{s}$ be the mean free scattering path (mean
distance travelled by a neutron between two successive collisions). The following equation is obtained:

$$
\lambda_{s}=\frac{\Sigma_{S}}{\Sigma_{t}^{2}} \approx \frac{1}{\Sigma_{S}} \text { in a slight absorbant medium }
$$

The number of collisions per second is $v / \lambda_{s}=v \Sigma_{S}$, and over a time interval $\Delta t$, the number of collisions undergone is: $v \Sigma_{S} \Delta t$. The energy loss for the continuous process is written as:

$$
v \Sigma_{S} \Delta t d E=v \Sigma_{S} E \xi d t
$$

The number of neutrons that reach energy $E$ by slowing down during time interval $d t$ and per $\mathrm{cm}^{3}$ of medium is:

$$
n(E) v \Sigma_{S} E \xi d t
$$

Thus, the slowing down density is:

$$
q(E)=\frac{n(E) v \Sigma_{S} E \xi d t}{d t}=n(E) v \Sigma_{S} E \xi
$$

Since $\Phi(E)=n(E) v$, the following equation is:

$$
\begin{equation*}
\text { Fermi slowing-down model: } q(E)=\xi \Sigma_{S} E \Phi(E) \tag{12.16}
\end{equation*}
$$

The time necessary to slow down a neutron from an energy of about 2 MeV to 0.0253 eV can be computed in continuous slowing-down theory in a graphite reactor by (Poulter 1963, p. 73):

$$
t=\int_{0.0253 e V}^{2 M e V} \frac{\lambda_{s}}{\xi v} \frac{d E}{E}=\frac{\overline{\lambda_{s}}}{\xi}\left(\frac{1}{v_{t h}}-\frac{1}{v_{0}}\right) \approx 1.510^{-4} \mathrm{~s}
$$

With $\overline{\lambda_{s}}=2.6 \mathrm{~cm}$ the mean scattering distance in graphite. The mean lethargy gain for carbon is $\xi=0.158, v_{t h}=2200 \mathrm{~m} . \mathrm{s}^{-1}$ and $v_{0}=19560 \mathrm{~km} . \mathrm{s}^{-1}$. The thermalization time, which is much longer and during which the neutron undergoes elastic scattering, should be added to this time. In pure graphite ( $\sigma_{c}=0.004$ barn, $\rho_{c}=1.7 \mathrm{~g} . \mathrm{cm}^{-3}$, thus $\Sigma_{c}=3.410^{-4} \mathrm{~cm}^{-1}$ ), the scattering time is $\ell_{\infty}=1 /$ $\left(v \Sigma_{c}\right)=13.4 \quad 10^{-3} \mathrm{~s}$. Since only $10 \%$ of the absorption occurs in graphite (it occurs chiefly in the fuel), the neutron lifetime decreases to $\ell_{\infty} \approx 10^{-3} \mathrm{~s}$.

### 12.7.3 Application to Neutron Diffusion

Using lethargy, $u$, the slowing-down density without up-scattering in energy is written as:

$$
q(u) \equiv \int_{-\infty}^{u} d u^{\prime} \int_{0}^{\infty} d u^{\prime \prime} \Sigma_{S}\left(u^{\prime} \rightarrow u^{\prime \prime}\right) \Phi\left(u^{\prime}\right)
$$

and by the definition of the scattering cross section, which is the integral of the differential scattering cross section $\Sigma_{S}(u)=\int_{u}^{\infty} \Sigma_{S}\left(u \rightarrow u^{\prime}\right) d\left(u^{\prime}\right)$, the following identity is obtained by differentiating $q(u)$ :

$$
\frac{\partial q(u)}{\partial u} \equiv \Sigma_{S}(u) \Phi(u)-\int_{-\infty}^{u} \Sigma_{S}\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime}
$$

The term $\int_{-\infty}^{u} \Sigma_{S}\left(u^{\prime} \rightarrow u\right) \Phi\left(u^{\prime}\right) d u^{\prime}$ is usually denoted as $\rho(u)$ or $R[\Phi(u)]$ that includes the slowing-down density operator $R$, the arrival density at lethargy $u$. The diffusion equation in lethargy is written as:

$$
D(u) \Delta \Phi(u)-(\underbrace{\Sigma_{a}(u)+\Sigma_{S}(u)}_{\Sigma_{t}(u)}) \Phi(u)+\rho(u)+S(u)=0
$$

i.e., using the expression $\partial q(u) / \partial u$ (Clark and Hansen 1964, p. 151; Bekurts and Wirtz 1964, p. 145):

$$
D(u) \Delta \Phi(u)-\Sigma_{a}(u) \Phi(u)-\frac{\partial q(u)}{\partial u}+S(u)=0
$$

Using the Fermi model to express $\Phi(u)$ in terms of $q(u)$, the equation obtained is:

$$
\frac{D(u)}{\xi \Sigma_{S}(u)} \Delta q(u)-\frac{\partial q(u)}{\partial u}+S(u)=0
$$

By neglecting the lethargy width of the fission spectrum $S(u)$, the equation for Fermi age is obtained by setting:

$$
d \tau=\frac{D(u)}{\xi \Sigma_{S}(u)} d u
$$

that is:

$$
\begin{equation*}
\text { Equation for Fermi age: } \Delta q(\tau)=\frac{\partial q(\tau)}{\partial \tau} \quad \text { with } \quad q(u=0)=\delta(\vec{r}) \tag{12.17}
\end{equation*}
$$

The quantity $\tau$ has the same dimensions as a surface area, but the equation for the age is similar to the heat equation where $\tau$ is equivalent to a time, thus the name Fermi age:

$$
\tau=\int_{0}^{u} \frac{D(u)}{\xi \Sigma_{S}(u)} d u=\int_{E}^{E_{0}} \frac{D(E)}{\xi \Sigma_{S}(E)} \frac{d E}{E}
$$

Several mathematical methods are used to solve the age equation by adapting the solutions to the heat conduction problem (Crank 1975). In the general case (significant absorption), the slowing-down density is proportional to the flux in terms of the scattering and absorption cross sections:

$$
q(E)=\left(\begin{array}{lll}
\xi & \Sigma_{S}+x & \Sigma_{a}
\end{array}\right) \Phi(u)
$$

If $x=0$ the Fermi model is obtained.
If $x=\xi \quad q(E)=\xi \Sigma_{t} \Phi(u)$, the Wigner model, described in Chap. 4, is obtained.
If $x=\gamma=\frac{\xi}{2 \int_{0}^{\infty} P(v) v d v}$ with $P(v)=P\left(u^{\prime} \rightarrow u\right)= \begin{cases}\frac{e^{-\left(u-u^{\prime}\right)}}{1-\alpha} & 0 \leq u-u^{\prime} \leq \varepsilon \\ 0 & \text { else }\end{cases}$
corresponds to the Greuling-Goertzel model that satisfies the first two moments of the slowing-down kernel $R(u)$.

### 12.7.4 Relation Between Fermi Age and Time

It should be pointed out that $d E /(\xi E)$ is the number of collisions that causes the neutron to travel from $E$ to $E-d E . \lambda_{s}=1 / \Sigma_{s}$ being the mean free scattering path, it can be inferred that $d E /\left(\xi E \Sigma_{S}\right)$ is the distance travelled by the neutron between two scattering collisions, i.e. the distance $v d t$. Since the increase in age is given by:

$$
d \tau=\frac{D(E)}{\xi \Sigma_{S}(E)} \frac{d E}{E}=D(E) v d t
$$

the age at a given energy is obtained by integrating over time:

$$
\tau(E)=\int_{0}^{t} D(E) v d t
$$

By setting a mean coefficient over the slowing-down period ${\overline{D_{0}}}_{\left[\mathrm{cm}^{2} / \mathrm{s}\right]}=$ $\frac{1}{t} \int_{0}^{t} D(E) v d t$, it can be shown that:

$$
\tau=\overline{D_{0}} t
$$

If a neutron is tracked up to $E_{t h}$, the Fermi age tends towards $\tau_{t h}$. Hence, the age is equivalent to a surface area that increases as the neutron slows down. It represents in a sense a scattering "smear" that is centered about the birth point of the neutron, although the path followed by the latter is in three dimensions. The greater the Fermi age, the further away a neutron may scatter from its origin. This value is thus essential for the calculation of the leakage effect during slowing down (Table 12.1).

In the case of water (light or heavy), the continuous age theory cannot be applied ideally (since water contains hydrogen for which the energy lost by slowing down at each collision can be very significant, in contradiction to Fermi's hypothesis). The values given in the table above are experimental points. It can be shown that the mean square distance travelled in a straight line from the source to the point at which thermal energy is reached is given by $\bar{r}^{2}=6 \cdot \tau$ in a homogeneous medium without leakage.

Let us consider a point source emitting neutrons in the fast spectrum at $E_{0}$ in a moderating medium. The number of collisions undergone by a neutron to reach $E_{t h}$ is tracked. Hence, the spreading of neutrons in space can be "visualized". If $r$ is the shortest distance from the source to the point t which the neutron reaches thermal energy $E_{t h}$, it can be shown that the mean square value of $r$ is given by (Fig. 12.16):

$$
\bar{r}^{2}=6 \cdot \tau_{t h}
$$

Table 12.1 Thermal age for some usual moderators

| Moderator at $20^{\circ} \mathrm{C}$ | $\tau_{t h:}$ age $\left(\mathrm{cm}^{2}\right)$ at thermal energy |
| :--- | :--- |
| Light water $\mathrm{H}_{2} \mathrm{O}$ | 33 |
| Beryllium | 98 |
| Beryllium oxide | 105 |
| Heavy water $\mathrm{D}_{2} \mathrm{O} 1.1 \mathrm{~g} / \mathrm{cm}^{3}$ | 120 |
| Graphite (carbon) | 350 |

Fig. 12.16 Sphere of radius
$r$ centered on S


### 12.7.5 Link Between the Age Theory and Diffusion Theory

(Ferziger and Zweifel 1966, p. 231; Stephenson 1954, p. 145).
The mono-energy theory of reactors (thermal diffusion equation) simplifies the slowing down phase. The age theory provides the required corrections. By definition, the thermal neutron source is $q\left(\tau_{t h}\right)$ where $q$ is the slowing down density. Neutron capture during slowing down is taken accounted for by escape probability factor $p$. Thus, the thermal neutron source is written as:

$$
S_{t h}=p q\left(\tau_{t h}\right)
$$

The proportion of fast neutrons emitted by absorption of a thermal neutron is $k_{\infty} / p$ since this number is multiplied by $p$ during slowing down to obtain $k_{\infty}$ thermal neutrons. The fast neutron source is expressed as:

$$
\underset{(\text { fast })}{S_{0}(\vec{r})=q_{(u=0, \vec{r})}=\frac{k_{\infty}}{p} \underbrace{\sum_{a_{t h}} \Phi_{t h}(\vec{r})}_{\begin{array}{c}
\text { Thermal } \\
\text { absorption } \\
\text { rate }
\end{array}}}
$$

associated with the Fermi age equation:

$$
\Delta q(\tau, \vec{r})=\frac{\partial q(\tau, \vec{r})}{\partial \tau}
$$

which can be integrated by separating the space and age variables (this hypothesis is only valid for a bare homogeneous reactor):

$$
q(\tau, \vec{r})=T(\tau) R(\vec{r})
$$

Thus: $\frac{\Delta R(\vec{r})}{R(\vec{r})}=\frac{1}{T(\tau)} \frac{d T(\tau)}{d \tau}=c s t=-B_{g}^{2}$
since $T(\tau)$ is obviously a decreasing function.

$$
\text { Hence: } \quad q(\tau, \vec{r})=T_{(u=0)} \cdot R(\vec{r}) \cdot e^{-B_{g}^{2} \tau}
$$

The constant $T_{(u=0)}$ is determined using $q_{(u=0, \vec{r})}: T_{(u=0)} R(\vec{r})=\frac{k_{\infty}}{p} \sum_{a_{t h}} \Phi(\vec{r})$

$$
\text { Therefore: } \quad q(\tau, \vec{r})=\frac{k_{\infty}}{p} \Sigma_{a_{t h}} \Phi_{t h}(\vec{r}) e^{-B_{g}^{2} \tau}
$$

Since the thermal neutron source is given by:

$$
S_{t h}=p q\left(\tau_{t h}, \vec{r}\right)=k_{\infty} \Sigma_{a_{t h}} \Phi_{t h}(\vec{r}) e^{-B_{g}^{2} \tau_{t h}}
$$

The diffusion equation for thermal neutrons is expressed as:

$$
D_{t h} \Delta \Phi_{t h}-\Sigma_{a_{t h}} \Phi_{t h}+k_{\infty} \Sigma_{a_{t h}} \Phi_{t h} e^{-B_{g}^{2} \tau_{t h}}=0
$$

The thermal neutron flux satisfies the fundamental mode equation:

$$
\Delta \Phi_{t h}(\vec{r})+B_{g}^{2} \quad \Phi_{t h}(\vec{r})=0
$$

thereby leading to the criticality condition with geometrical buckling $B_{g}^{2}$, and thermal scattering area $L^{2}$ :

$$
-\frac{D_{t h} B_{g}^{2}}{\sum_{a_{t h}}}-1+k_{\infty} e^{-B_{g}^{2} \tau_{t h}}=0
$$

which can be expressed in the conventional form:
Criticality condition in mono-energy diffusion theory corrected by age theory:

$$
\begin{equation*}
\frac{k_{\infty} e^{-B_{g}^{2} \tau_{t h}}}{1+L^{2} B_{g}^{2}}=1 \tag{12.18}
\end{equation*}
$$

Factor $e^{-B_{g}^{2} \tau_{t h}}$ is the non-leakage probability of the reactor in the absence of absorption. Factor $p e^{-B_{g}^{2} \tau_{t h}}$ is the probability of a neutron completing the slowing down process without leakage (either by absorption or by leaving the reactor). This property is ideal in the absence of slowing down in light nuclei (due to the hypotheses imposed by age theory: small mean lethargy gain $\xi$ ). The migration area is given by:

$$
M^{2}=\frac{\int_{0}^{\infty} D(E) \varphi_{0}(E) d E}{\int_{0}^{\infty} \Sigma_{a}(E) \varphi_{0}(E) d E}
$$

where $\varphi_{0}(E)$ is the solution to: $D B_{g}^{2} \varphi_{0}+\Sigma_{a} \varphi_{0}=\underbrace{p q\left(\tau_{t h}\right)}$
thermal neutron source
In age theory and in an infinite scattering medium: $\tau_{t h}+L^{2}=\frac{1}{6} \overline{r^{2}}=M^{2}{ }_{\left(B_{g}=0\right)}$
whereas for a finite medium: $M^{2} \approx L^{2}+\tau_{t h}$
For large reactors ( $B_{g}^{2} \ll 1$ ), expansion of the exponential term into Taylor series at first order leads to:

$$
e^{-B_{g}^{2} \tau_{t h}} \approx 1-B_{g}^{2} \tau_{t h}
$$

Thereby giving an effective multiplication factor:
$k_{e f f}=k_{\infty} \frac{e^{-B_{g}^{2} \tau_{t h}}}{1+L^{2} B_{g}^{2}} \approx k_{\infty} \frac{1-B_{g}^{2} \tau_{t h}}{1+L^{2} B_{g}^{2}} \approx \frac{k_{\infty}}{\left(1+B_{g}^{2} \tau_{t h}\right)\left(1+L^{2} B_{g}^{2}\right)} \approx \frac{k_{\infty}}{1+\left(L^{2}+\tau_{t h}\right) B_{g}^{2}}$
Hence, we find the expression for a bare homogeneous reactor: $k_{e f f}=\frac{k_{\infty}}{1+M^{2} B_{g}^{2}}$.

### 12.7.6 Two-Energy Group Equation in Fermi Age Theory

In the chapter on diffusion, the following equation was established:

$$
\overline{r^{2}}=6 L^{2}=6 \frac{D}{\Sigma_{a}}
$$

For a fast neutron, by analogy, the following equation is obtained in age theory:

$$
\begin{gathered}
\overline{r_{1}^{2}}=6 \frac{D_{1}}{\Sigma_{a_{1}}}=6 \tau_{t h} \\
\text { Thus: } \tau_{t h}=\frac{D_{1}}{\Sigma_{a_{1}}}
\end{gathered}
$$

Let $\Phi_{t h}$ be the thermal flux, the thermal group becoming group 2 in two-group theory $\left(\Phi_{t h}=\Phi_{2}\right)$. Let $\Sigma_{a_{2}} \Phi_{2}$ be the number of thermal neutrons absorbed. By definition of the fuel multiplication factor $\eta, \eta \Sigma_{a_{2}} \Phi_{2}$ fast neutrons are emitted immediately after fission. Thus, given that some fast neutrons may induce fission reactions (especially for ${ }^{238} U$ ), $\varepsilon \eta \Sigma_{a_{2}} \Phi_{2}$ fast neutrons are obtained. $\varepsilon$ is the fast fission factor. Thus, the fast neutron source is given by:

$$
S_{1}=\eta \varepsilon \quad \Sigma_{a_{2}} \Phi_{2}
$$

With no loss during slowing down (escape probability factor $p$ ) and by absorption in structural elements (thermal use factor $f$ ), the thermal flux source is $\Sigma_{a_{1}} \Phi_{1}$ (i.e. the fast absorption rate). The cross section $\Sigma_{a_{1}}$ can be broken down into capture (very small at fast energy), fission (small in the fast energy range) and transfer towards group $2 \Sigma_{r}$, which is the main component. Accounting for neutrons lost during slowing down and in structures for an infinite medium, the scheme (Blaquière 1962) for the absorption of a thermal neutron is the following (Fig. 12.17):

After one cycle, the resulting source is:

$$
S_{2}=p f \Sigma_{a, 1} \Phi_{1}
$$

The expression for the transfer cross section can also be written as:

Fig. 12.17 Blaquière scheme for a thermal neutron


$$
\Sigma_{r}=p f \Sigma_{a, 1}
$$

Thus, the two-group equations are:

$$
\left\{\begin{array}{l}
D_{1} \Delta \Phi_{1}-\Sigma_{a, 1} \Phi_{1}+\varepsilon \eta \Sigma_{a, 2} \Phi_{2}=0 \\
D_{2} \Delta \Phi_{2}-\Sigma_{a, 2} \Phi_{2}+p f \Sigma_{a, 1} \quad \Phi_{1}=0
\end{array}\right.
$$

By injecting: $\Sigma_{a, 1}=\frac{D_{1}}{\tau_{t h}}$ and $\left\{\begin{array}{l}\Delta \Phi_{1}+B_{g}^{2} \\ \Delta \Phi_{2}+B_{g}^{2}=0 \\ \Phi_{2}=0\end{array}\right.$ in cases close to the fundamental mode for a bare homogeneous reactor, the following equations are found:

$$
\left\{\begin{array} { l } 
{ D _ { 1 } B _ { g } ^ { 2 } \Phi _ { 1 } - \frac { D _ { 1 } } { \tau _ { t h } } \Phi _ { 1 } + \varepsilon \eta \Sigma _ { a , 2 } \Phi _ { 2 } = 0 } \\
{ D _ { 2 } B _ { g } ^ { 2 } \Phi _ { 2 } - \Sigma _ { a , 2 } \Phi _ { 2 } + p f \frac { D _ { 1 } } { \tau _ { t h } } \Phi _ { 1 } = 0 }
\end{array} \text { or } \left\{\begin{array}{l}
\left(1+B_{g}^{2} \tau_{t h}\right) \Phi_{1}-\frac{\varepsilon \eta \tau_{t h}}{D_{1}} \Sigma_{a, 2} \Phi_{2}=0 \\
-\frac{p f D_{1}}{\Sigma_{a, 2} \tau_{t h}} \Phi_{1}+(1+B_{g}^{2} \underbrace{\frac{D_{2}}{\sum_{a, 2}}}_{L^{2}}) \Phi_{2}=0
\end{array}\right.\right.
$$

In this equation, there is the thermal scattering area: $L^{2}=D_{2} / \Sigma_{a_{2}}$. The equation for the geometrical buckling $B_{g}^{2}$ is obtained by cancelling the determinant of the above system to allow for an infinite number of solutions $\left(\Phi_{1}, \Phi_{2}\right)$, i.e.:

$$
\left(1+B_{g}^{2} \tau_{t h}\right)\left(1+B_{g}^{2} L^{2}\right)=\underbrace{\eta \varepsilon p f}_{k_{\infty}}
$$

This is the four-factor formula illustrated in Chap. 11:

$$
k_{\infty}=\eta \varepsilon p f
$$

thus: $\tau_{t h} L^{2}\left(B_{g}^{2}\right)^{2}+\left(\tau_{t h}+L^{2}\right) B_{g}^{2}+1-k_{\infty}=0$

The two roots of this equation, positive $\alpha^{2}$ and negative $-\beta^{2}$, are written as:

$$
\left\{\begin{aligned}
\alpha^{2} & =\frac{-\left(\tau_{t h}+L^{2}\right)+\sqrt{\left(\tau_{t h}+L\right)^{2}-4 \tau_{t h} L^{2}\left(1-k_{\infty}\right)}}{2 \tau_{t h} L^{2}} \\
-\beta^{2} & =\frac{-\left(\tau_{t h}+L^{2}\right)-\sqrt{\left(\tau_{t h}+L\right)^{2}-4 \tau_{t h} L^{2}\left(1-k_{\infty}\right)}}{2 \tau_{t h} L^{2}}
\end{aligned}\right.
$$

Material buckling corresponds to positive solution $\alpha^{2}$. The criticality condition is written as:

$$
B_{g}^{2}=\alpha^{2}
$$

where $\alpha^{2}$ depends only on the composition of the medium. It can be noticed that the effective multiplication factor is:

Effective multiplication factor in the age theory:

$$
\begin{equation*}
k_{\text {eff }}=\frac{k_{\infty}}{\left(1+B_{g}^{2} \tau_{t h}\right)\left(1+B_{g}^{2} L^{2}\right)} \tag{12.19}
\end{equation*}
$$

For large reactors $\left(B_{g}^{2} \ll 1\right)$ :

$$
k_{e f f} \approx \frac{k_{\infty}}{\left(1+\left(\tau_{t h}+L^{2}\right) B_{g}^{2}\right)}=\frac{k_{\infty}}{\left(1+M^{2} B_{g}^{2}\right)}
$$

By way of illustration, historically, the British Magnox reactors, moderated by graphite and cooled by gas, were calculated using the cylindrical geometry equations with an anisotropic diffusion coefficient (Poulter 1963, p. 51):

$$
\left\{\begin{array}{l}
D_{1, r}\left(\frac{\partial^{2} \Phi_{1}}{\partial r^{2}}+\frac{1}{r} \frac{\partial \Phi_{1}}{\partial r}\right)+D_{1, z} \frac{\partial^{2} \Phi_{1}}{\partial z^{2}}-\Sigma_{a, 1} \Phi_{1}+\eta \varepsilon p f \Sigma_{a, 2} \Phi_{2}=0 \\
D_{2, r}\left(\frac{\partial^{2} \Phi_{2}}{\partial r^{2}}+\frac{1}{r} \frac{\partial \Phi_{2}}{\partial r}\right)+D_{2, z} \frac{\partial^{2} \Phi_{2}}{\partial z^{2}}-\Sigma_{a, 2} \Phi_{2}+\Sigma_{1 \rightarrow 2} \Phi_{1}=0
\end{array}\right.
$$

and

$$
k_{e f f}=\frac{k_{\infty}}{\left(1+\alpha^{2} \tau_{t h, z}+\beta^{2} \tau_{t h, r}\right)\left(1+\alpha^{2} L_{z}^{2}+\beta^{2} L_{r}^{2}\right)}
$$

where:

$$
\alpha=\frac{\pi}{\text { Effective height }} \text { and } \beta=\frac{j_{0,1}}{\text { Effective radius }}
$$

### 12.7.7 Age-Diffusion Theory

Honeck and Ott in (Van Antwerpen 1954, p. 107).
The theory known as age-diffusion theory consists in approximating the Boltzmann equation in the slowing down domain by:

$$
\left\{\begin{array}{l}
\operatorname{div} \vec{J}(\vec{r}, u)+\Sigma_{t}(\vec{r}, u) \Phi(\vec{r}, u)=-\frac{\partial q(\vec{r}, u)}{\partial u}+S(\vec{r}, u) \\
\overrightarrow{\operatorname{grad}} \Phi(\vec{r}, u)+3 \Sigma_{t r}(\vec{r}, u) \vec{J}(\vec{r}, u)=0
\end{array}\right.
$$

The term $S(\vec{r}, u)$ consists of the fission sources and the inelastic scattering sources at high energy. $q(\vec{r}, u)=\xi \Sigma_{s} \Phi(\vec{r}, u)$ is the slowing down density and $-\partial$ $q(\vec{r}, u) / \partial u$ is the slowing down source due to elastic scattering. In the thermal range within which the neutron is no longer slowed down but rather exchanges energy with the materials in the core, the following equations are written:

$$
\left\{\begin{array}{l}
\operatorname{div} \vec{J}(\vec{r}, u)+\Sigma_{t}(\vec{r}, u) \Phi(\vec{r}, u)=q\left(\vec{r}, u_{t h}\right) \\
\overrightarrow{\operatorname{grad}} \Phi(\vec{r}, u)+3 \Sigma_{t r}(\vec{r}, u) \vec{J}(\vec{r}, u)=0
\end{array}\right.
$$

A multi-group approach is possible by integrating the first system of equations on the lethargy range $\left[u_{g}, u_{g+1}\right]$, by dropping the indices for space for concision, and by assuming that the inelastic scatterings are negligible, thus giving a fissiononly source:
$\left\{\begin{array}{l}-D_{g}\left(u_{g+1}-u_{g}\right) \Delta \Phi_{g}+\Sigma_{t}^{g} \Phi_{g}\left(u_{g+1}-u_{g}\right)=q\left(u_{g}\right)-q\left(u_{g+1}\right)+\left(u_{g+1}-u_{g}\right) \chi_{g} \sum_{g^{\prime}} \nu \Sigma_{f}^{g^{\prime}} \Phi_{g^{\prime}} \\ \vec{J}_{g}=-\frac{1}{3 \Sigma_{t r}^{g}} \overrightarrow{\operatorname{grad}} \Phi_{g} \equiv-D_{g} \overrightarrow{\operatorname{grad}} \Phi_{g}\end{array}\right.$
This system can be written in the usual form:

$$
\left\{\begin{array}{l}
-D_{g} \Delta \Phi_{g}+\Sigma_{t}^{g} \Phi_{g}=\sum_{g^{\prime}=1}^{g} \sum_{g^{\prime} \rightarrow g}^{g} \Phi_{g^{\prime}}+\chi_{g} \sum_{g^{\prime}} \nu \Sigma_{f}^{g^{\prime}} \Phi_{g^{\prime}} \\
-D_{t h} \Delta \Phi_{t h}+\Sigma_{t}^{t h} \Phi_{t h}=\sum_{g^{\prime}=1}^{G} \Sigma_{g^{\prime} \rightarrow t h}^{g} \Phi_{g^{\prime}}
\end{array}\right.
$$

### 12.8 Multi-Group Diffusion

Two characteristic zones are distinguished:

- the slowing down domain in which neutrons may be emitted by fission or by slowing down to lower groups (thus, from a higher energy),


Fig. 12.18 Transfer matrix

- the thermalization zone in which there is no production by fission but energy is transferred between the upper and lower groups.

This can be represented by a scattering matrix that depends on the individual isotope. The heavier the isotope, the sparser the matrix will be since light isotopes will efficiently slow down neutrons, thereby filling the lower triangular part of the matrix, with group 1 being the fastest group, corresponding to the position at the top left of the matrix (Fig. 12.18).

The multi-group diffusion equations are expressed as follows:

$$
\begin{cases}-D_{g} \Delta \Phi_{g}+\Sigma_{t}^{g} \Phi_{g}=\sum_{g^{\prime}=1}^{g} \sum_{g^{\prime} \rightarrow g}^{g} \Phi_{g^{\prime}}+\chi_{g} \sum_{g^{\prime}} \nu \Sigma_{f}^{g^{\prime}} \Phi_{g^{\prime}} & \text { slowing down } \\ -D_{g} \Delta \Phi_{g}+\Sigma_{t}^{g} \Phi_{g}=\sum_{g^{\prime}=g_{c}}^{G} \Sigma_{g^{\prime} \rightarrow g}^{g} \Phi_{g^{\prime}} & \text { thermalization }\end{cases}
$$

Group $g_{c}$ corresponds to the cut-off beyond which there is no up-scattering in energy, which is worth 2.7 eV for a thermalized reactor. In the thermalization zone, the neutrons can gain energy by collision with matter (up-scattering).

### 12.9 Reactor Kinetics in One-Group Diffusion Theory with Source

Until now, only the static diffusion equation has been considered. We will here deal with the time-dependent flux for a bare homogeneous reactor. The time-dependent diffusion equation is written as:

$$
\begin{equation*}
\frac{1}{v} \frac{\partial \Phi(\vec{r}, t)}{\partial t}-D \Delta \Phi(\vec{r}, t)+\Sigma_{a} \Phi(\vec{r}, t)=S(\vec{r}, t)+\nu \Sigma_{f} \Phi(\vec{r}, t) \tag{12.20}
\end{equation*}
$$

The term $\partial \Phi(\vec{r}, t) /(v \partial t)$ represents variation in the neutron population $\partial n(\vec{r}, t) / \partial t$. The basis of eigenfunctions of the Laplace operator, $\Phi_{k}(\vec{r})$, is used to project the flux solution as:

$$
\Phi(\vec{r}, t)=\sum_{k} \varphi_{k}(t) \Phi_{k}(\vec{r}) \text { with } \varphi_{k}(t)=\frac{\int_{V} \Phi(\vec{r}, t) \Phi_{k}(\vec{r}) d \vec{r}}{\int_{V} \overline{\Phi_{k}}(\vec{r}) \Phi_{k}(\vec{r}) d \vec{r}}
$$

If an orthonormal basis is used, the terms $\int_{V} \overline{\Phi_{k}}(\vec{r}) \Phi_{k}(\vec{r}) d \vec{r}=1$ can be cancelled. Similarly, the source that does not depend on the flux is also projected as:

$$
S(\vec{r}, t)=\sum_{k} s_{k}(t) \Phi_{k}(\vec{r})
$$

By inserting these expansions in Eq. (12.20) then multiplying by the eigenfunction $\overline{\Phi_{k}}(\vec{r})$, it is possible to make use of the orthogonality properties of the eigenfunctions shown at the beginning of the chapter, producing a set of differential equations for the time-dependent coefficients:

$$
\begin{aligned}
& \int_{V} d \vec{r} \overline{\Phi_{k}}(\vec{r})[\frac{1}{v} \sum_{k} \frac{\partial \varphi_{k}(t)}{\partial t} \Phi_{k}(\vec{r})-D \sum_{k} \varphi_{k}(t) \underbrace{\Delta \Phi_{k}(\vec{r})}_{-B_{k}^{2} \Phi_{k}(\vec{r})}+\left(\Sigma_{a}-\nu \Sigma_{f}\right) \sum \varphi_{k}(t) \Phi_{k}(\vec{r})] \\
& =\int_{V} \overline{\Phi_{k}}(\vec{r}) \sum_{k} s_{k}(t) \Phi_{k}(\vec{r}) d \vec{r} \\
& \frac{1}{v} \frac{\partial \varphi_{k}(t)}{\partial t}+\left(D B_{k}^{2}+\Sigma_{a}-\nu \Sigma_{f}\right) \quad \varphi_{k}(t)=s_{k}(t)
\end{aligned}
$$

The general solution to this differential equation is written by setting $\lambda_{k} / \nu=$ $D B_{k}^{2}+\Sigma_{a}-\nu \Sigma_{f}$ :

$$
\varphi_{k}(t)=\alpha(t) e^{-\lambda_{k} t}
$$

Using the method of variation of parameters, the equation finally obtained is:

$$
\varphi_{k}(t)=\left[C+v \int_{0}^{t} s_{k}(t) e^{+\lambda_{k} t}\right] e^{-\lambda_{k} t}
$$

Using any flux as the initial condition $\Phi(\vec{r}, 0)=\sum_{k} \varphi_{k}(0) \Phi_{k}(\vec{r})$, the value of the constant is obtained as $C=\varphi_{k}(0)$. In the particular case of a non-multiplying medium ( $\nu \Sigma_{f}=0$ ) without source $\left(s_{k}(t)=0\right)$, the flux is a sum of decreasing exponential terms for which that having the smallest coefficient (corresponding to $\lambda_{1}$ ) becomes the prevailing term as time increases:

$$
\Phi(\vec{r}, t)=\sum_{k} \varphi_{k}(0) e^{-\lambda_{k} t} \Phi_{k}(\vec{r}) \quad \underset{t \rightarrow \infty}{\approx} \varphi_{k}(0) e^{-\lambda_{1} t} \Phi_{0}(\vec{r})
$$

The flux decays proportionally to a fundamental mode. This result can be used to measure the diffusion coefficient and the absorption cross section of the medium [Horowitz-Raievski method (Atoms for peace 1955, Volume V, p. 46)]. For the same non-multiplying medium, if the source is constant over time, i.e. the coefficients $s_{k}$ do not vary with time, the flux tends towards a constant flux as time tends to infinity:

Flux in a non-multiplying medium with constant source :
$\Phi(\vec{r}, t)=\sum_{k}\left(\frac{s_{k}}{D B_{k}^{2}+\Sigma_{a}}+\left(\varphi_{k}(0)-\frac{s_{k}}{D B_{k}^{2}+\Sigma_{a}}\right) e^{-\lambda_{k} t}\right) \Phi_{k}(\vec{r}) \underset{t \rightarrow \infty}{\approx} \sum_{k} \frac{s_{k}}{D B_{k}^{2}+\Sigma_{a}} \Phi_{k}(\vec{r})$

This result is valid even if the medium is sub-multiplying ( $k_{\infty}<1$ ), in which case, $\Sigma_{a}$ is substituted by $\Sigma_{a}-\nu \Sigma_{f}=\Sigma_{a}\left(1-k_{\infty}\right) \geq 0$ in the previous formula, and hence $\lambda_{1}$ is still positive. The formulae show that the permanent state reached is such that the flux level is higher than that for a non-multiplying medium with constant source. If the medium is over-multiplying ( $k_{\infty}>1$ ), the condition for a positive $\lambda_{1}$ (or any positive $\lambda_{k}$ in general) leads to a minimum value of $B_{1}^{2}$, which is another way of writing the criticality condition:

$$
B_{1}^{2}>\frac{\Sigma_{a}\left(k_{\infty}-1\right)}{D}
$$

If $B_{1}^{2}$ is lower than this critical value, then:

Fig. 12.19 Evolution of flux in the presence of a source


$$
\frac{\lambda_{1}}{v}=D B_{1}^{2}+\Sigma_{a}\left(1-k_{\infty}\right)<0 \text { and } e^{-\lambda_{1} t} \underset{t \rightarrow+\infty}{\rightarrow}+\infty
$$

The flux increases in an exponential manner, following a dominant term that is proportional to the fundamental mode. The term $B_{1}^{2}$ corresponds to the square of the geometrical buckling of the considered volume and $D B_{1}^{2}$ to the neutron leakage term through the outer surface of the volume. The reactor can remain globally sub-critical as long as leakage compensates for the production term, which is proportional to $k_{\infty}-1$.

If the reactivity becomes so great that the other values of $\lambda_{k}$ become negative, the associated harmonics can be taken into account, but they remain insignificant compared to the fundamental mode. This result is very important for the physics of the phenomenon and we will discuss the flux expansion as the product of a timedependent function and the fundamental mode in the chapter on neutron kinetics (point kinetics model). If the reactor is critical, the flux varies linearly with time in the presence of a source (Fig. 12.19).

### 12.10 Source Calculation: Extension to Multi-Group Conditions

In the previous section, the behavior of a reactor in the presence of independent sources that are not coupled to the flux (in contrast to the fission sources) was studied with time dependence. In a sub-critical case, the flux level tends towards a constant level depending on the source. The two-energy group approach illustrates
this fact. In an infinite reactor (with no leakage), the two-group diffusion equations with a source term (placed in the fast group) are written as:

$$
\left\{\begin{array}{l}
\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) \Phi_{1}=\nu \Sigma_{f 1} \Phi_{1}+\nu \Sigma_{f 2} \Phi_{2}+S \\
\Sigma_{a 2} \Phi_{2}=\Sigma_{1 \rightarrow 2} \Phi_{1}
\end{array}\right.
$$

This linear system is solved in a conventional manner by writing the system in the form:

$$
\left\{\begin{array}{l}
\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}-\nu \Sigma_{f 1}\right) \Phi_{1}-\nu \Sigma_{f 2} \Phi_{2}=S \\
\Sigma_{1 \rightarrow 2} \Phi_{1}-\Sigma_{a 2} \Phi_{2}=0
\end{array}\right.
$$

for which the determinant is:

$$
\text { Det }=\left|\begin{array}{cc}
\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}-\nu \Sigma_{f 1}\right) & -\nu \Sigma_{f 2} \\
\Sigma_{1 \rightarrow 2} & -\Sigma_{a 2}
\end{array}\right|=\left(k_{\infty}-1\right) \Sigma_{a 2}\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right)
$$

Introducing for two energy groups the value $k_{\infty}$ :

$$
k_{\infty}=\frac{\nu \Sigma_{f 1} \Sigma_{a 2}+\nu \Sigma_{f 2} \Sigma_{1 \rightarrow 2}}{\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) \Sigma_{a 2}}
$$

which is itself obtained from solution of the system:

$$
\left\{\begin{array}{l}
\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right) \Phi_{1}=\frac{\nu \Sigma_{f 1} \Phi_{1}+\nu \Sigma_{f 2} \Phi_{2}}{k_{\infty}} \\
\Sigma_{a 2} \Phi_{2}=\Sigma_{1 \rightarrow 2} \Phi_{1}
\end{array}\right.
$$

It is seen that there is no stationary solution to the problem if $k_{\infty}=1$ for the intrinsically critical reactor, since $D e t=0$. The flux couple ( $\Phi_{1}, \Phi_{2}$ ) that satisfies this source system is given by:

$$
\left\{\begin{array}{l}
\Phi_{1}=\frac{\left|\begin{array}{cc}
S & -\nu \Sigma_{f 2} \\
0 & -\Sigma_{a 2}
\end{array}\right|}{\text { Det }}=\frac{-\Sigma_{a 2} S}{\left(k_{\infty}-1\right) \Sigma_{a 2}\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right)} \\
\Phi_{2}=\frac{\left|\begin{array}{cc}
\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}-\nu \Sigma_{f 1}\right) & S \\
\Sigma_{1 \rightarrow 2} & 0
\end{array}\right|}{\text { Det }}=\frac{-\Sigma_{1 \rightarrow 2} S}{\left(k_{\infty}-1\right) \Sigma_{a 2}\left(\Sigma_{a 1}+\Sigma_{1 \rightarrow 2}\right)}
\end{array} .\right.
$$

for which the only physical solutions for positive flux are those for the reactors where the determinant is negative, i.e. sub-critical reactors such that $k_{\infty}<1$. In this frame, the flux varies linearly with the source. If the reactor were finite, the fast and thermal leakage terms, $-D_{1} \Delta \Phi_{1}$ and $-D_{2} \Delta \Phi_{2}$ respectively, must be taken into account in the diffusion equations, which is equivalent to substituting the
absorption cross section $\Sigma_{a}$ by $\Sigma_{a}+D B_{g}^{2}$, and by modeling the Laplace term by a fundamental mode in the previous calculations. A similar logic can be applied and substitute $k_{\infty}$ by $k_{e f f}$. If the reactor is infinite and over-critical, $k_{\infty}>1$, no permanent flux solution is possible and the problem should be dealt with in the time-dependent framework using the flux projection on spherical harmonics for instance. The flux then increases continuously, adopting the dominant shape of the fundamental mode.

## Chapter 13 Neutron Reflectors

The physics of a reactor is significantly improved by surrounding it with a neutron reflector, i.e. structural elements that enclose the fissile zone, rather than just a bare reactor with a vacuum around it. It will also be seen that the properties of this reflector impact the neutron economy of the reactor. In 1939, Francis Perrin was the first to suggest the idea of surrounding a reactor with graphite blocks to reduce the size of the fissile zone. This idea was successfully implemented by Enrico Fermi for the CP1 pile, then for the first French reactor with heavy water, Zoé [acronym for Zero energy, Oxide, Heavy water ["Eau lourde" in French], (Nahmias 1953, p. 134; Lefebvre 2002, p. 35)]. The neutron reflector of $P W R$ is mainly constituted of water and steel. It reflects back thermal neutrons towards the core and leads to an "economy" (or a gain) in fissile matter compared to a bare core. Another advantage is that it greatly improves the form factor by flattening the power distribution. Calculation of the neutron properties of the reflector is a key step in the calculation scheme for a reactor, a topic not often discussed in the standard references, ${ }^{1}$ despite the fact that a significant amount of theoretical research work has been carried out on this subject.

### 13.1 Some Mathematical Considerations on Reflectors

Let $\Omega_{R}$ be a reflector in contact with the fuel material $\Omega_{C}$ (Fig. 13.1), comprising a non-multiplying medium $\left(\Sigma_{f}=0\right)$ in which the Poisson equation with no source is solved in diffusion theory as follows:

[^271]Fig. 13.1 Fuel/reflector geometry


$$
-\operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}\right)+\Sigma_{t g} \Phi_{g}=\sum_{g^{\prime} \rightarrow g} \Sigma_{g g^{\prime}} \Phi_{g^{\prime}}
$$

It can be shown that ${ }^{2}$ if $\Phi$ is the solution to the partial derivative equation in $\Omega_{R}$ without source, and with Dirichlet conditions:

$$
\left\{\begin{array}{c}
-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi)+\Sigma \Phi=0 \\
\Phi=\Phi_{\text {boundary }}
\end{array}\right.
$$

or with von Neumann boundary conditions:

$$
\left\{\begin{array}{c}
-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi)+\Sigma \Phi=0 \\
-D \frac{\partial \Phi}{\partial n}=J_{\text {boundary }}
\end{array}\right.
$$

there exists an operator called the Poincaré-Steklov ${ }^{3}$ operator R such that: $-D \frac{\partial \Phi}{\partial n}=R\left[\Phi_{\partial \Omega_{R}}\right]$.

[^272]
## Picture 13.1a Henri

Poincaré (Public domain)


Picture 13.1b Vladimir
A. Steklov (source: website of the city of Kharkov, Public domain)


This implies that the behavior of the solution at the boundary $\partial \Omega_{C} \cap \partial \Omega_{R}$ is totally characterized by operator $R$ at the boundaries of the domain. The Poincar-é-Steklov operator depends only on $\Omega_{R}$ and the neutron properties of the reflector, but not on the state of the domain outside $\Omega_{R}$, i.e. the nature of the fuel (Picture 13.1a and 13.1b).

The normal derivative of the flux at a point on $\partial \Omega_{C} \cap \partial \Omega_{R}$ depends on the values of $\Phi$ for the whole boundary (and not only on $\Phi$ at the considered position, where only a $l D$ geometry allows this simplification). It should be noted that the operator $R$ is linear since the initial partial derivative equation system is linear. It will be shown below that this operator R employs the reflector as the boundary condition of the active core. This operator is represented by a transfer matrix denoted as $\mathfrak{R}$ which relates the net current to the flux:

$$
\vec{J} \cdot \vec{n}=J^{-}-J^{+}=\mathfrak{R}[\Phi]
$$

### 13.2 Reflectors in Diffusion Theory

### 13.2.1 Case of the Slab Reactor Surrounded by an Infinite Reflector

Let us consider a slab reactor with:

- diffusion coefficient $D_{c}$,
- macroscopic absorption cross section $\Sigma_{a, c}$,
- production cross section $v \Sigma_{f, c}$,
- scattering area $L_{c}^{2}$,
- multiplication coefficient in infinite medium $k_{\infty, c}$.

The reactor is surrounded by an infinite reflector medium of:

- diffusion coefficient $D_{r}$,
- macroscopic absorption cross section $\Sigma_{a, r}$,
- scattering area $L_{r}^{2}$,
- attenuation coefficient $\kappa_{r}$.

The goal is to study the impact of the reflector on the neutron flux solution in the whole reactor (Stacey 2001, p. 66). The solution in fundamental mode in the core (indexed by $c$ ) as illustrated previously is given as:

$$
\Phi_{c}(x)=\Phi_{c}(0) \cos \left(B_{c} x\right) \quad \text { with } B_{c}=\sqrt{\frac{k_{\infty, c}-1}{M_{c}^{2}}}
$$

The thermal diffusion equation in the reflector is written as:

$$
-D_{r} \Delta \Phi_{r}(x)+\Sigma_{a, r} \Phi_{r}(x)=0
$$

which will be expressed in its canonical form using the migration area of the reflector $M_{r}^{2} \equiv D_{r} / \Sigma_{a, r} \equiv 1 / \kappa_{r}^{2}$ where $\kappa_{r}$ has the same role as an attenuation coefficient (Fig. 13.2):

Diffusion equation in a reflector :

$$
\begin{equation*}
\Delta \Phi_{r}(x)-\frac{1}{M_{r}^{2}} \Phi_{r}(x)=\Delta \Phi_{r}(x)-\kappa_{r}^{2} \Phi_{r}(x)=0 \tag{13.1}
\end{equation*}
$$

The solution in the reflector is written as:

Fig. 13.2 Neutron flux in a slab reactor reflected by an infinite reflector


$$
\Phi_{r}(x)=\Phi_{d}^{+} e^{k_{r}\left(x-\frac{a}{2}\right)}+\Phi_{d}^{-} e^{-k_{r}\left(x-\frac{a}{2}\right)}
$$

thus simplifying the modeling of boundary conditions at infinity. On the right $\Phi_{r}(\infty)=0$, thus $\Phi_{d}^{+}=0$. On the left, the following equation is written:

$$
\Phi_{r}(x)=\Phi_{g}^{+} e^{k_{r}\left(x+\frac{a}{2}\right)}+\Phi_{g}^{-} e^{-k_{r}\left(x+\frac{a}{2}\right)}
$$

Since $\Phi_{r}(-\infty)=0$, it can be deduced that $\Phi_{g}^{-}=0$. The flux continuity at the right boundary at $a / 2$ is expressed as:

$$
\Phi_{c}(a / 2)=\Phi_{c}(0) \cos \left(B_{c} \frac{a}{2}\right)=\Phi_{d}^{-} .
$$

Similarly, on the left boundary at $-a / 2$ : thus $\Phi_{g}^{+}=\Phi_{g}^{-}$. The continuity of the current (given by Fick's law $\vec{J}=-D \overrightarrow{\operatorname{grad} \Phi}$ ) is written as:
$D_{c} \Phi_{c}(0) B_{c} \sin \left(B_{c} \frac{a}{2}\right)=D_{r} \Phi_{d}^{-} \kappa_{r} \quad$ Current continuity on the right at $a / 2$ :
On the left:
$-D_{c} \Phi_{c}(0) B_{c} \sin \left(-B_{c} \frac{a}{2}\right)=D_{r} \Phi_{g}^{+} \kappa_{r} \quad$ Current continuity of the left at $-a / 2$ :
which corresponds to the same equation since:

$$
\Phi_{g}^{+}=\Phi_{d}^{-}=\frac{D_{c} \Phi_{c}(0) B_{c} \sin \left(B_{c} \frac{a}{2}\right)}{D_{r} \kappa_{r}}
$$

Finally, the following three equations governing flux are obtained, depending on the medium for which it is being computed:

$$
\begin{cases}\Phi_{c}(x)=\Phi_{c}(0) \cos \left(B_{c} x\right) & \text { in the fuel } \\ \Phi_{r}(x)=\Phi_{c}(0) \sin \left(B_{c} \frac{a}{2}\right) \frac{B_{c}}{\kappa_{r}} \frac{D_{c}}{D_{r}} e^{-\kappa_{r}\left(x-\frac{a}{2}\right)} \quad \text { in the reflector on the right } \\ \Phi_{r}(x)=\Phi_{c}(0) \sin \left(B_{c} \frac{a}{2}\right) \frac{B_{c}}{\kappa_{r}} \frac{D_{c}}{D_{r}} e^{\kappa_{r}\left(x+\frac{a}{2}\right)} \quad \text { in the reflector on the left }\end{cases}
$$

Given the symmetries of the problem, flux is maximum at the center of the reactor $\Phi_{c}(0)=\Phi_{\text {max }}$, and these equations can be expressed as:

Flux for fuel and reflector in slab geometry :

$$
\left\{\begin{array}{c}
\Phi_{c}(x)=\Phi_{\max } \cos \left(B_{c} x\right)  \tag{13.2}\\
\Phi_{r}(x)=\Phi_{\max } \sin \left(B_{c} \frac{a}{2}\right) \frac{B_{c}}{\kappa_{r}} \frac{D_{c}}{D_{r}} e^{-\kappa_{r}\left(|x|-\frac{a}{2}\right)}
\end{array}\right.
$$

Flux expression in the reflector can also be written as follows, using the flux continuity equation at the interface, $x=a / 2$ :

$$
\begin{aligned}
\Phi_{r}\left(\frac{a}{2}\right)=\Phi_{\max } \sin \left(B_{c} \frac{a}{2}\right) \frac{B_{c}}{\kappa_{r}} \frac{D_{c}}{D_{r}} e^{-\kappa_{r}\left(\frac{a}{2}-\frac{a}{2}\right)} & =\Phi_{\max } \sin \left(B_{c} \frac{a}{2}\right) \frac{B_{c}}{\kappa_{r}} \frac{D_{c}}{D_{r}} \\
& =\Phi_{c}\left(\frac{a}{2}\right)=\Phi_{\max } \cos \left(B_{c} \frac{a}{2}\right)
\end{aligned}
$$

Hence: $\Phi_{r}(x)=\Phi_{c}\left(\frac{a}{2}\right) e^{-\kappa_{r}\left(|x|-\frac{a}{2}\right)}$
The flux in the reflector is obtained by simply extrapolating the flux value in the fuel at the interface using a decreasing exponential function. This result is useful in several practical applications as will be illustrated below. The criticality condition is obtained by dividing each term of the current continuity equation by that of the flux: $D_{c} B_{c} \tan \left(B_{c} a / 2\right)=D_{r} \kappa_{r}$, which can be expressed as:

Criticality condition of a slab reactor with an infinite reflector:

$$
\begin{equation*}
\frac{a}{2}=\frac{1}{B_{c}} \arctan \left(\frac{D_{r} \kappa_{r}}{D_{c} B_{c}}\right) \tag{13.3}
\end{equation*}
$$

It may be seen that the term on the left depends only on geometrical parameters whereas the term on the right depends on the material properties of the core and the reflector, a condition which has been previously expressed as "geometrical buckling $=$ material buckling." However, $a / 2$ is not the geometrical buckling of a slab. It will be shown that surrounding a reactor with a reflector decreases neutron leakage (the reflector directs neutrons back towards the core), thereby leading to a decrease in the reactor size, and hence economy in terms of fissile material. Let us consider a bare and infinite slab reactor (surrounded by a vacuum), as studied previously and of thickness $\tilde{a}$. If $\delta$ is the c to zero, then $\tilde{a}=a+2 \delta$. The bare reactor is critical if $\tilde{\mathrm{a}}$ satisfies the criticality condition, i.e.:

$$
B_{c}^{2}=\frac{k_{\infty, c}-1}{M_{c}^{2}}=\frac{\pi^{2}}{\widetilde{\mathrm{a}}^{2}}
$$

If $\delta$ is introduced in the criticality condition of the reflected reactor $D_{c} B_{c} \tan \left(B_{c} a / 2\right)=D_{r} \kappa_{r}$ using $a=\tilde{a}-2 \delta$, and given that $B_{c} \tilde{a}=\pi$, the following equation is obtained:

$$
\tan \left(B_{c} \frac{a}{2}\right)=\tan \left(B_{c} \frac{\tilde{a}}{2}-B_{c} \delta\right)=\tan \left(\frac{\pi}{2}-B_{c} \delta\right)=\operatorname{cotan}\left(B_{c} \delta\right)
$$

Besides, assuming that the core is large (around a meter, such that $B_{c}=\pi / \tilde{a}$ $<10^{-2} \mathrm{~cm}^{-1}$ ), then the approximation $\operatorname{cotan}\left(B_{c} \delta\right)=1 / B_{c} \delta-B_{c} \delta / 3+\ldots$ is valid for the cotangent if $B_{c} \delta .<\pi$. Inserting this expansion in Taylor series into the criticality condition gives:

$$
D_{c} B_{c}\left(\frac{1}{B_{c} \delta}-\frac{B_{c} \delta}{3}+\ldots\right)=D_{r} \kappa_{r} \quad \text { i.e. } \quad \delta \approx \frac{D_{c}}{D_{r} \kappa_{r}}
$$

at the first order. Hence, the approximate value of $\delta$, called reflector economy:

$$
\begin{equation*}
\text { Reflector economy: } \quad \delta \approx \frac{D_{c}}{D_{r} \kappa_{r}}=\frac{D_{c}}{\sqrt{D_{r} \Sigma_{a, r}}} \tag{13.4}
\end{equation*}
$$

This expression represents the economy of fissile material resulting from the presence of a reflector. Further, the smaller the absorption cross section of the reflector, the larger will be this economy. Conversely, if the reflector were a perfect neutron absorber, no neutrons would be directed back towards the core. However, the reflector is even more efficient if the diffusion coefficient is smaller. A diffusion coefficient that is too large tends to allow neutrons to leak further away, and they are thus unable to be redirected into the core. Indeed, the larger $\delta$ is, the smaller will be the size of the reactor. In the field of fast reactors, the term reflector gain is employed, which is different from reflector economy. The gain is the difference at critical state between the extrapolated length and the real geometrical dimension of the fuel lattice. ${ }^{4}$ This reflector gain is of the order of 15 cm for the PHENIX and SUPERPHENIX reactors (sodium-cooled fast reactors), but can reach up to 35 cm for high power gas-cooled fast reactors.

[^273]
### 13.2.2 Reflected Homogeneous Slab Reactor

Let us now consider the same core (multiplying medium) composed of a slab of thickness $a$ and defined by $D_{c}, \Sigma_{a, c}, \nu \Sigma_{f, c}, k_{\infty, c}, M_{c}^{2}$, with a reflector of thickness $b$ on either side of the core, and defined by $D_{r}, \Sigma_{a, r}, \kappa_{r}^{2}=\Sigma_{a, r} / D_{r}$ or $M_{r}^{2}=D_{r} / \Sigma_{a, r}$. The reflector is a non-multiplying medium, scattering and weakly absorbing, placed at the core periphery to limit the number of neutrons leaking outside (Fig. 13.3).

Some of the neutrons leaving the core are reflected back into it after some scattering collisions. The reflector acts as a source of thermal neutrons with respect to the core. The equations governing the flux are:

- Fuel: $\frac{d^{2} \Phi}{d x^{2}}+B_{c}^{2} \Phi_{c}(x)=0 \quad 0 \leq|x| \leq \frac{a}{2}$
- Reflector: $\frac{d^{2} \Phi}{d x^{2}}-\kappa_{r}^{2} \Phi_{r}(x)=0 \quad \frac{a}{2} \leq|x| \leq \frac{a}{2}+b$
- Flux continuity: $\Phi_{c}(a / 2)=\Phi_{r}(a / 2)$
- Current continuity: $-D_{c}\left(\frac{d \Phi_{c}}{d x}\right)_{x=a / 2}=-D_{r}\left(\frac{d \Phi_{r}}{d x}\right)_{x=a / 2}$
- Boundary conditions: $\Phi_{r}\left(\frac{a}{2}+b\right)=0$
with $B_{c}^{2} \equiv\left(k_{\infty, c}-1\right) / M_{c}^{2}$. This notation with the square sign implies that the medium is over-multiplying, i.e. $k_{\infty, c} \geq 1$. The equations for $x<0$ are obtained by symmetry. It should be pointed out that the current continuity at the core/reflector interface implies a discontinuity on the derivative of the flux at the same interface. $\kappa_{r}^{2}=\Sigma_{a, r} / \mathrm{D}_{r}$ is written as a square to visualize a positive quantity that is dimensionally homogeneous to the inverse of a surface area. It can be shown that there is no solution if $B_{c}^{2} \leq 0$, which is physically explained as follows: the reflector limits


Fig. 13.3 One-group neutron flux in a slab reactor reflected by a finite reflector
leakage terms but does not decrease them to zero. Thus, a critical system is obtained only if $k_{\infty, c}>1$, so as to compensate for these leakages. The solutions are of the form:

$$
\left\{\begin{aligned}
\Phi_{c}(x) & =\Phi_{\sin } \sin \left(B_{c} x\right)+\Phi_{\cos } \cos \left(B_{c} x\right) \\
\Phi_{r}(x)=\Phi_{+} e^{\kappa_{r} x}+\Phi_{-} e^{-\kappa_{r} x} & =\Phi_{c h}^{+} \operatorname{ch}\left(\kappa_{r}\left(\frac{a}{2}+b-x\right)\right)+\Phi_{s h}^{+} \operatorname{sh}\left(\kappa_{r}\left(\frac{a}{2}+b-x\right)\right)
\end{aligned}\right.
$$

The flux in the fuel is symmetrical in $x$, thus:

$$
\Phi_{c}(x)=\Phi_{c}(0) \quad \cos \left(B_{c} x\right)
$$

The flux in the reflector is also symmetrical but defined in a piecemeal manner. Using the condition that the flux cancels out at the exterior boundaries on the right and left, the following is obtained:

On the right: $\Phi_{r}\left(\frac{a}{2}+b\right)=\Phi_{c h}^{+} \operatorname{ch}(0)+\Phi_{s h}^{+} \operatorname{sh}(0)=\Phi_{c h}^{+}=0$
Thus on the right: $\Phi_{r}(x)=\Phi_{s h}^{+} \operatorname{sh}\left(\kappa_{r}\left(\frac{a}{2}+b-x\right)\right)$
On the left, the flux is written using hyperbolic functions:

$$
\Phi_{r}(x)=\Phi_{c h}^{-} \operatorname{ch}\left(\kappa_{r}\left(-\frac{a}{2}-b-x\right)\right)+\Phi_{s h}^{-} \operatorname{sh}\left(\kappa_{r}\left(-\frac{a}{2}-b-x\right)\right)
$$

On the left: $\Phi_{r}\left(-\frac{a}{2}-b\right)=\Phi_{c h}^{-} \operatorname{ch}(0)+\Phi_{s h}^{-} \operatorname{sh}(0)=\Phi_{c h}^{-}=0$
Therefore, the flux in the reflector is:

$$
\Phi_{r}(x)=\Phi_{s h}^{-} \operatorname{sh}\left(\kappa_{r}\left(-\frac{a}{2}-b-x\right)\right)
$$

The constants $\Phi_{s h}^{+}, \Phi_{s h}^{-}$and $\Phi_{c}(0)$ remain to be determined. The two conditions that express the continuity of the flux and that of the current at $x=a / 2$ become as follows, using the reflector flux on the right:

$$
\begin{cases}\Phi_{c}(0) \cos \left(B_{c} a / 2\right)=\Phi_{s h}^{+} \operatorname{sh} \kappa_{r} b & \text { Flux continuity at a/2 } \\ \Phi_{c}(0) D_{c} B_{c} \sin \left(B_{c} a / 2\right)=\Phi_{s h}^{+} D_{r} \kappa_{r} c h \kappa_{r} b & \text { Current continuity }\end{cases}
$$

It can also be deduced that: $\Phi_{s h}^{+}=\Phi_{c}(0) \frac{\cos \left(B_{c} a / 2\right)}{s h \kappa_{r} b}$
The same calculation on the left for $x=-a / 2$ leads to:

$$
\begin{cases}\Phi_{c}(0) \cos \left(-B_{c} a / 2\right)=\Phi_{s h}^{-} \operatorname{sh}\left(-\kappa_{r} b\right) & \text { Flux continuity at }-\mathrm{a} / 2 \\ -\Phi_{c}(0) D_{c} B_{c} \sin \left(-B_{c} a / 2\right)=-\Phi_{s h}^{-} D_{r} \kappa_{r} c h\left(-\kappa_{r} b\right) & \text { Current continuity }\end{cases}
$$

From which: $\Phi_{s h}^{-}=-\Phi_{c}(0) \frac{\cos \left(B_{c} a / 2\right)}{s h c_{r} b}$, it can be seen that $\Phi_{s h}^{-}=-\Phi_{s h}^{+}$
The term-wise ratio of these two equations leads to the same compatibility condition. This criticality condition can be used to determine the physical properties of the core that turns the system critical when the geometry is defined, or to
compute the critical thickness of the core when the physical properties are defined. In any event, there is an infinite number of solutions, the first being the fundamental mode, with the others being the higher harmonics.
$\left\{\begin{array}{l}\Phi_{c}(x)=\Phi_{c}(0) \cos \left(B_{c} x\right) \\ \Phi_{r}(x)=\Phi_{c}(0) \frac{\cos \left(B_{c} a / 2\right)}{\operatorname{sh} \kappa_{r} b} \operatorname{sh}\left(\kappa_{r}\left(\frac{a}{2}+b-x\right)\right) \quad \text { in the reflector on the right } \\ \Phi_{r}(x)=\Phi_{c}(0) \frac{\cos \left(B_{c} a / 2\right)}{\operatorname{sh} \kappa_{r} b} \operatorname{sh}\left(\kappa_{r}\left(\frac{a}{2}+b+x\right)\right) \quad \text { in the reflector on the left }\end{array}\right.$
Using $\Phi_{c}(0)=\Phi_{\max }$, these equations can also be written as:
Flux in fuel and finite reflector in a slab geometry:

$$
\left\{\begin{array}{cl}
\Phi_{c}(x)=\Phi_{\max } & \cos \left(B_{c} x\right)  \tag{13.5}\\
\Phi_{r}(x)=\Phi_{\max } \frac{\cos \left(B_{c} a / 2\right)}{\operatorname{sh} \kappa_{r} b} & \operatorname{sh}\left(\kappa_{r}\left(\frac{a}{2}+b-|x|\right)\right)
\end{array}\right.
$$

By dividing the flux continuity equation term-wise by the current continuity equation, the following criticality condition is obtained:

Criticality condition for the reflected slab reactor:

$$
\begin{equation*}
D_{c} B_{c} \tan \left(B_{c} \frac{a}{2}\right)=D_{r} \kappa_{r} \operatorname{coth}\left(\kappa_{r} b\right) \tag{13.6}
\end{equation*}
$$

This transcendental equation does not separate the geometrical elements (geometrical buckling that would depend on the lengths $a$ and $b$ ) from the material properties (material buckling). The hypotheses of "large reactor size" or "large reflector" could be used to simplify the hyperbolic tangent and cotangent terms using Taylor expansions for simplified calculations.

### 13.2.3 Case of an Infinite Cylindrical Reactor Surrounded by an Infinite Reflector

Let us consider an infinite cylinder of radius $R$ for which the flux solution was previously determined, and which is now surrounded by an infinite non-multiplying reflector:

$$
\left\{\begin{array}{l}
\Delta \Phi_{c}(r)+B_{c}^{2} \Phi_{c}(r)=\frac{d^{2} \Phi_{c}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{c}(r)}{d r}+B_{c}^{2} \Phi_{c}(r)=0 \\
\Delta \Phi_{r}(r)-\kappa_{r}^{2} \Phi_{r}(r)=\frac{d^{2} \Phi_{r}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{r}(r)}{d r}-\kappa_{r}^{2} \Phi_{r}(r)=0
\end{array}\right.
$$

The flux and current continuity at the interface is expressed as:

$$
\left\{\begin{array}{l}
\Phi_{c}(R)=\Phi_{r}(R) \\
\left(-D_{c} \operatorname{grad}\left(\Phi_{c}(r)\right)\right)_{R}=\left(-D_{r} \operatorname{grad}\left(\Phi_{r}(r)\right)\right)_{R}
\end{array}\right.
$$

The general solution for the modified Bessel equation for a core is given by:

$$
\Phi_{c}=\Phi_{J} J_{0}\left(B_{c} r\right)+\Phi_{Y} Y_{0}\left(B_{c} r\right)
$$

Where the core buckling is given by $B_{g}{ }^{2}=\lambda$ and, $J_{0}(r)$ and $Y_{0}(r)$ are the first and second kind zero-order Bessel function. $\Phi_{c}(0)$ must be finite $\left(=\Phi_{\max }\right)$. Since $Y_{0}(0)=-\infty, \Phi_{Y}=0$. The general solutions to the modified Bessel equation for a reflector with $I_{0}(r)$ and $K_{0}(r)$ are modified Bessel functions of the first and second kind at order 0 (Fig. 13.4):

$$
\Phi_{r}=\Phi_{I} I_{0}\left(\kappa_{r} r\right)+\Phi_{K} K_{0}\left(\kappa_{r} r\right)
$$

$\Phi_{r}(\infty)$ must be finite. Since $I_{0}(+\infty)=+\infty, \Phi_{I}=0$. The flux continuity at $R$ is expressed as:


Fig. 13.4 Axially-infinite cylinder, of radius $R$, reflected by an infinite reflector

$$
\Phi_{c}(R)=\Phi_{J} J_{0}\left(B_{c} R\right)=\Phi_{r}(R)=\Phi_{K} K_{0}\left(\kappa_{r} R\right)
$$

Thus: $\quad \frac{\Phi_{J}}{\Phi_{K}}=\frac{K_{0}\left(\kappa_{r} R\right)}{J_{0}\left(B_{c} R\right)}$
Current continuity is written as:

$$
\begin{aligned}
\left(-D_{c} \operatorname{grad}\left(\Phi_{c}(r)\right)\right)_{R} & =-D_{c}\left(-\Phi_{J} B_{c} J_{1}\left(B_{c} R\right)\right)=\left(-D_{r} \operatorname{grad}\left(\Phi_{r}(r)\right)\right)_{R} \\
& =-D_{r}\left(-\Phi_{K} \kappa_{r} K_{1}\left(\kappa_{r} R\right)\right)
\end{aligned}
$$

Finally, since $J_{0}(0)=1$, the coefficient $\Phi_{J}$ is simply the maximum flux $\Phi_{\max }$. The flux is given by:

$$
\begin{cases}\Phi_{c}(r)=\Phi_{\max } J_{0}\left(B_{c} r\right) & \text { in the core } \\ \Phi_{r}(r)=\Phi_{\max } \frac{J_{0}\left(B_{c} R\right)}{K_{0}\left(\kappa_{r} R\right)} K_{0}\left(\kappa_{r} r\right) & \text { in the reflector }\end{cases}
$$

The flux in the reflector can also be expressed under the form: $\Phi_{r}(r)=\Phi_{c}(R)$ $K_{0}\left(\kappa_{r} r\right) / K_{0}\left(\kappa_{r} R\right)$. Using the "large reactor" hypothesis, the Bessel function $K_{0}$ can be developed into series when $\kappa_{r} r$ is large:

$$
K_{n}(x) \approx \sqrt{\frac{\pi}{2 x}} e^{-x}\left[1+\frac{4 n^{2}-1^{2}}{1!8 x}+\frac{\left(4 n^{2}-1^{2}\right)\left(4 n^{2}-3^{2}\right)}{2!(8 x)^{2}}+\ldots\right]
$$

Hence:

$$
\begin{aligned}
& \Phi_{r}(r)=\Phi_{c}(R) \frac{\sqrt{\frac{\pi}{2 \kappa_{r} r}}}{\sqrt{\frac{\pi}{2 \kappa_{r} R}} e^{-\kappa_{r} r}\left[1+\frac{3}{8 \kappa_{r} r}+\ldots\right]} \\
& \quad \approx \Phi_{c}(R) \sqrt{\frac{R}{r} R}\left[1-\frac{1}{8 \kappa_{r} R}+\ldots\right] \\
& e^{-\kappa_{r}(r-R)}\left[1+\frac{4}{8 \kappa_{r} r}+\frac{3}{64\left(\kappa_{r} r\right)^{2}}\right]
\end{aligned}
$$

It should be noted that close to $R$, the approximation $\Phi_{r}(r) \approx \Phi_{c}(R) \quad e^{-\kappa_{r}(r-R)}$ is satisfactory for the flux in the reflector, thereby leading to the same formulation as for the slab reactor. The criticality condition is obtained by dividing the flux continuity equation by the current continuity equation:

Criticality condition for an infinitely-reflected cylindrical reactor:

$$
\begin{equation*}
D_{c} B_{c} \frac{J_{1}\left(B_{c} R\right)}{J_{0}\left(B_{c} R\right)}=D_{r} \kappa_{r} \frac{K_{1}\left(\kappa_{r} R\right)}{K_{0}\left(\kappa_{r} R\right)} \tag{13.7}
\end{equation*}
$$

In the case of the slab reactor, it will be shown that surrounding a reactor with a reflector decreases its size, leading to economy in fissile material. Let us consider a
bare (surrounded by a vacuum) infinite cylindrical reactor, as studied previously, of radius $\tilde{R}$. The distance at which the flux cancels out is denoted as $\delta$, and thus $\tilde{R}=R+\delta$. The bare reactor is critical if $\tilde{R}$ satisfies the criticality condition, i.e.:

$$
B_{c}^{2} \equiv \frac{k_{\infty, c}-1}{M_{c}^{2}}=\frac{j_{0,1}^{2}}{\widetilde{R}^{2}}
$$

If $\delta$ is introduced in the criticality condition for the reflected cylindrical reactor using the fact that $R=\tilde{R}-\delta$, and that $B_{c} \tilde{R}=j_{0,1}$, the following equation is obtained:

$$
D_{c} B_{c} \frac{J_{1}\left(B_{c} \widetilde{R}-B_{c} \delta\right)}{J_{0}\left(B_{c} \widetilde{R}-B_{c} \delta\right)}=D_{r} \kappa_{r} \frac{K_{1}\left(\kappa_{r} \widetilde{R}-\kappa_{r} \delta\right)}{K_{0}\left(\kappa_{r} \widetilde{R}-\kappa_{r} \delta\right)}
$$

The Bessel functions are developed into Taylor series and a recurrence relation is used to express the derivative of $J_{n}(x)$ as a function of $J_{n}(x)$ and $J_{n-1}(x)$ :

$$
\begin{aligned}
J_{1}\left(B_{c} \widetilde{R}-B_{c} \delta\right) & \approx J_{1}\left(B_{c} \widetilde{R}\right)-B_{c} \delta J_{1}^{\prime}\left(B_{c} \widetilde{R}\right) \\
& =J_{1}\left(j_{0,1}\right)-B_{c} \delta(-\frac{J_{1}\left(B_{c} \widetilde{R}\right)}{B_{c} \widetilde{R}}+\underbrace{J_{0}(\underbrace{B_{c} \widetilde{R}}_{j_{0,1}})}_{0}) \\
& =\left(1+\frac{\delta}{\widetilde{R}}\right) J_{1}\left(j_{0,1}\right)
\end{aligned}
$$

thus:

$$
\begin{gathered}
J_{0}\left(B_{c} \widetilde{R}-B_{c} \delta\right) \approx \underbrace{J_{0}(\underbrace{B_{c} \widetilde{R}}_{j_{0,1}})}_{0}-B_{c} \delta J_{0}^{\prime}\left(B_{c} \widetilde{R}\right)=-B_{c} \delta(-J_{1}(\underbrace{B_{c} \widetilde{R}}_{j_{0,1}})) \\
=B_{c} \delta J_{1}\left(j_{0,1}\right)
\end{gathered}
$$

Using the recurrence relation: $x K_{n}^{\prime}(x)=-n K_{n}(x)-x K_{n-1}(x)$

$$
\begin{gathered}
K_{1}\left(\kappa_{r} \widetilde{R}-\kappa_{r} \delta\right) \approx K_{1}\left(\kappa_{r} \widetilde{R}\right)-\kappa_{r} \delta K_{1}^{\prime}\left(\kappa_{r} \widetilde{R}\right) \\
=K_{1}\left(\kappa_{r} \widetilde{R}\right)-\kappa_{r} \delta\left(-\frac{K_{1}\left(\kappa_{r} \widetilde{R}\right)}{\kappa_{r} \widetilde{R}}-K_{0}\left(\kappa_{r} \widetilde{R}\right)\right) \\
=\left(1+\frac{\delta}{\widetilde{R}}\right) K_{1}\left(\kappa_{r} \widetilde{R}\right)+\kappa_{r} \delta K_{0}\left(\kappa_{r} \widetilde{R}\right) \\
K_{0}\left(\kappa_{r} \widetilde{R}-\kappa_{r} \delta\right) \approx K_{0}\left(\kappa_{r} \widetilde{R}\right)-\kappa_{r} \delta K_{0}^{\prime}\left(\kappa_{r} \widetilde{R}\right) \\
= \\
=K_{0}\left(\kappa_{r} \widetilde{R}\right)-\kappa_{r} \delta\left(-K_{1}\left(\kappa_{r} \widetilde{R}\right)\right)=K_{0}\left(\kappa_{r} \widetilde{R}\right)+\kappa_{r} \delta K_{1}\left(\kappa_{r} \widetilde{R}\right)
\end{gathered}
$$

By substituting the latter in the criticality condition, the following equation is obtained:

$$
\begin{aligned}
& \qquad D_{c} B_{c} \frac{\left(1+\frac{\delta}{\tilde{R}}\right) J_{1}\left(j_{0,1}\right)}{B_{c} \delta J_{1}\left(j_{0,1}\right)}=D_{r} \kappa_{r} \frac{\left(1+\frac{\delta}{\tilde{R}}\right) K_{1}\left(\kappa_{r} \widetilde{R}\right)+\kappa_{r} \delta K_{0}\left(\kappa_{r} \widetilde{R}\right)}{K_{0}\left(\kappa_{r} \widetilde{R}\right)+\kappa_{r} \delta K_{1}\left(\kappa_{r} \widetilde{R}\right)} \\
& \text { hence: } \frac{D_{c}}{D_{r} \kappa_{r}} K_{0}\left(\kappa_{r} \tilde{R}\right)=\delta\left(K_{1}\left(\kappa_{r} \tilde{R}\right)-\frac{D_{c}}{D_{r} \kappa_{r}} K_{0}\left(\kappa_{r} \tilde{R}\right) \frac{1}{\tilde{R}}-\frac{D_{c}}{D_{r}} K_{1}\left(\kappa_{r} \tilde{R}\right)\right)+ \\
& \delta^{2}\left(\frac{1}{\tilde{R}} K_{1}\left(\kappa_{r} \tilde{R}\right)+\kappa_{r} K_{0}\left(\kappa_{r} \tilde{R}\right)-\frac{1}{\tilde{R}} \frac{D_{c}}{D_{r}} K_{1}\left(\kappa_{r} \tilde{R}\right)\right)
\end{aligned}
$$

An exact evaluation of $\delta$ may be obtained from this quadratic equation. Using the "large reactor" hypothesis, which is expressed as $\delta \ll \tilde{R}$, and where $\kappa_{r} \tilde{R}$ is large enough, simplifies the equation by neglecting the terms in $\delta^{2}$. Using the expansion for sufficiently large values of $x$ :

$$
K_{n}(x) \approx \sqrt{\frac{\pi}{2 x}} e^{-x}\left[1+\frac{4 n^{2}-1^{2}}{1!8 x}+\frac{\left(4 n^{2}-1^{2}\right)\left(4 n^{2}-3^{2}\right)}{2!(8 x)^{2}}+\ldots\right]
$$

The following ratio can also be deduced $\frac{K_{1}(x)}{K_{0}(x)} \approx \frac{1+\frac{3}{8 x}+\ldots}{1+\frac{3}{8 x}+\ldots} \approx 1+\frac{4}{8 x}+\frac{3}{64 x^{2}}+\ldots \approx 1$
Hence: $\frac{D_{c}}{D_{r} \kappa_{r}} \frac{\left(1+\frac{\delta}{\tilde{R}}\right)}{\delta}=\frac{\left(1+\frac{\delta}{\tilde{R}}\right) \frac{K_{1}\left(\kappa_{r} \tilde{R}\right)}{K_{0}\left(\kappa_{r} \tilde{R}\right)}+\kappa_{r} \delta}{1+\kappa_{r} \delta \frac{K_{1}\left(\kappa_{r} \tilde{R}\right)}{K_{0}\left(\kappa_{r} \tilde{R}\right)}} \approx \frac{\left(1+\frac{\delta}{\tilde{R}}\right)+\kappa_{r} \delta}{1+\kappa_{r} \delta}$
Reflector economy for the cylindrical reactor:

$$
\begin{equation*}
\frac{D_{c}}{D_{r} \kappa_{r}}-\approx \delta \frac{1+\frac{\kappa_{r} \delta}{\left(1+\frac{\delta}{R}\right)}}{1+\kappa_{r} \delta} \approx \delta\left(1+\kappa_{r} \delta\left(1-\frac{\delta}{\widetilde{R}}\right)\left(1-\kappa_{r} \delta\right)\right) \tag{13.8}
\end{equation*}
$$

hence, at first order in cylindrical geometry, $\delta \approx D_{c} /\left(D_{r} \kappa_{r}\right)$. If the terms at higher orders of $\delta$ are ignored, the formula for the reflector economy in slab geometry is thus found: $\delta \approx D_{c} /\left(D_{r} \kappa_{r}\right) \equiv D_{c} / \sqrt{D_{r} \Sigma_{a, r}}$. This result is very logical since for an external observer located close to its surface, the cylinder appears to be a plane. The same result would also be found for a sphere.

Technology, Engineering and Safety (1963, p. 509) provides several illustrations of fuel economy in terms of critical mass for different geometries. We have selected the case of a homogeneous spherical solution of uranium (93.2\% enrichment in ${ }^{235}$ $U$ ) and water (Fig. 13.5). It can be seen that the presence of a water reflector leads to a saving of more than twice the amount of fuel required to reach the critical mass.

Criticality control of fissile materials (1968, p. 3) presents several plots of the critical volumes for aqueous spherical solutions of $\mathrm{UO}_{2}$ and/or $\mathrm{PuO}_{2}$ reflected by water [see (Contrôle de la criticalité 1961)].


Fig. 13.5 Comparison of critical masses for a bare homogeneous spherical reactor and a sphere reflected by water [adapted from W.H. Roach in (Technology, Engineering and Safety 1963)] [ x -axis: kg of U235 per liter of solution, y -axis: critical mass in kg ]

### 13.2.4 Case of an Infinite Cylindrical Reactor with a Finite Reflector

### 13.2.4.1 Monocinetic Calculation

Let us consider an infinite cylinder of radius $R$, for which the flux was determined earlier, and surrounded by a non-multiplying reflector:

$$
\left\{\begin{array}{l}
\Delta \Phi_{c}(r)+B_{c}^{2} \Phi_{c}(r)=\frac{d^{2} \Phi_{c}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{c}(r)}{d r}+B_{c}^{2} \Phi_{c}(r)=0 \\
\Delta \Phi_{r}(r)-\kappa_{r}^{2} \Phi_{r}(r)=\frac{d^{2} \Phi_{r}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{r}(r)}{d r}-\kappa_{r}^{2} \Phi_{r}(r)=0
\end{array}\right.
$$

The flux and current continuity at the interface, coupled with the null flux hypothesis in the reflector at its boundary, are expressed as:

$$
\left\{\begin{array}{l}
\Phi_{c}\left(R_{c}\right)=\Phi_{r}\left(R_{c}\right) \\
\Phi_{r}\left(R_{r}\right)=0 \\
\left(-D_{c} \operatorname{grad}\left(\Phi_{c}(r)\right)\right)_{R_{c}}=\left(-D_{r} \operatorname{grad}\left(\Phi_{r}(r)\right)\right)_{R c}
\end{array}\right.
$$

As in the previous case, the general solution of the modified Bessel equation for the core is:

$$
\Phi_{c}=\Phi_{J} J_{0}\left(B_{c} r\right)+\Phi_{Y} Y_{0}\left(B_{c} r\right)
$$

where core buckling is given by $B_{c}{ }^{2}=\lambda_{c} . \Phi_{c}(0)$ must be finite $\left(=\Phi_{\max }\right)$. Since $Y_{0}(0)=-\infty, \Phi_{Y}=0$. The general solution to the modified Bessel equation for the reflector is (Fig. 13.6):

Fig. 13.6 Axially-infinite cylinder of radius $R_{c}$ surrounded by a reflector of radius $R_{r}$


$$
\Phi_{r}=\Phi_{I} I_{0}\left(\kappa_{r} r\right)+\Phi_{K} K_{0}\left(\kappa_{r} r\right)
$$

In the present case, $\Phi_{I}$ cannot be cancelled due to the flux being finite at infinity. The system of equation for the flux is thus written as:

$$
\left\{\begin{array}{cc}
\Phi_{c}(r)=\Phi_{J} J_{0}\left(B_{c} r\right) & \frac{d \Phi_{c}(r)}{d r}=-\Phi_{J} B_{c} J_{1}\left(B_{c} r\right) \\
\Phi_{r}(r)=\Phi_{I} I_{0}\left(\kappa_{r} r\right)+\Phi_{K} K_{0}\left(\kappa_{r} r\right) & \frac{d \Phi_{r}(r)}{d r}=\Phi_{I} \kappa_{r} I_{1}\left(\kappa_{r} r\right)-\Phi_{K} \kappa_{r} K_{1}\left(\kappa_{r} r\right)
\end{array}\right.
$$

The continuity equations and boundary conditions are expressed as:

$$
\left\{\begin{array}{l}
\Phi_{c}\left(R_{c}\right)=\Phi_{J} J_{0}\left(B_{c} R_{c}\right)=\Phi_{r}\left(R_{c}\right)=\Phi_{I} I_{0}\left(\kappa_{r} R_{c}\right)+\Phi_{K} K_{0}\left(\kappa_{r} R_{c}\right) \\
\Phi_{r}\left(R_{r}\right)=0=\Phi_{I} I_{0}\left(\kappa_{r} R_{r}\right)+\Phi_{K} K_{0}\left(\kappa_{r} R_{r}\right) \\
-D_{c} \Phi_{J}\left(-B_{c} J_{1}\left(B_{c} R_{c}\right)\right)=-D_{r}\left(\Phi_{I} \kappa_{r} I_{1}\left(\kappa_{r} R_{r}\right)-\Phi_{K} \kappa_{r} K_{1}\left(\kappa_{r} R_{r}\right)\right)
\end{array}\right.
$$

Finally, since $J_{0}(0)=1, \Phi_{J}=\Phi_{\max }$, the flux may be written as:

$$
\left\{\begin{array}{c}
\Phi_{c}(r)=\Phi_{\max } J_{0}\left(B_{c} r\right) \\
\Phi_{r}(r)=\Phi_{\max }\binom{\frac{J_{0}\left(B_{c} R_{c}\right) K_{0}\left(\kappa_{r} R_{r}\right)}{K_{0}\left(\kappa_{r} R_{r}\right) I_{0}\left(\kappa_{r} R_{c}\right)-K_{0}\left(\kappa_{r} R_{c}\right) I_{0}\left(\kappa_{r} R_{r}\right)}}{+\frac{J_{0}\left(B_{c} R_{c}\right) I_{0}\left(\kappa_{r} R_{r}\right)}{K_{0}\left(\kappa_{r} R_{c}\right) I_{0}\left(\kappa_{r} R_{r}\right)-K_{0}\left(\kappa_{r} R_{r}\right) I_{0}\left(\kappa_{r} R_{c}\right)} K_{0}\left(\kappa_{r} r\right)}
\end{array}\right.
$$

The criticality condition is obtained by replacing $A, D$ and $E$ by their full formulae in the current continuity equation:

$$
D_{c} \Phi_{J}\left(B_{c} J_{1}\left(B_{c} R_{c}\right)\right)=-D_{r}\left(\Phi_{I} \kappa_{r} I_{1}\left(\kappa_{r} R_{r}\right)-\Phi_{K} \kappa_{r} K_{1}\left(\kappa_{r} R_{r}\right)\right)
$$

Hence:
Criticality condition for an infinite cylindrical reactor reflected by a finite reflector:

$$
\begin{gather*}
D_{c} B_{c} J_{1}\left(B_{c} R_{c}\right)=-D_{r} \frac{J_{0}\left(B_{c} R_{c}\right) K_{0}\left(\kappa_{r} R_{r}\right)}{K_{0}\left(\kappa_{r} R_{r}\right) I_{0}\left(\kappa_{r} R_{c}\right)-K_{0}\left(\kappa_{r} R_{c}\right) I_{0}\left(\kappa_{r} R_{r}\right)} \kappa_{r} I_{1}\left(\kappa_{r} R_{r}\right)  \tag{13.9}\\
+D_{r} \frac{J_{0}\left(B_{c} R_{c}\right) I_{0}\left(\kappa_{r} R_{r}\right)}{K_{0}\left(\kappa_{r} R_{c}\right) I_{0}\left(\kappa_{r} R_{r}\right)-K_{0}\left(\kappa_{r} R_{r}\right) I_{0}\left(\kappa_{r} R_{c}\right)} \kappa_{r} K_{1}\left(\kappa_{r} R_{r}\right)
\end{gather*}
$$

As seen earlier, this equation relates the geometrical data of the reactor to its material data. This highly complex transcendental equation may be simplified using the "large reactor" hypothesis with the usual considerations ( $B_{c} \ll 1$ ).

### 13.2.4.2 Two-Energy Group Calculation

The previous results may be improved with two energy groups by extending the boundary conditions, and solving the following equations with the usual notations, without the $r$ index for the reflector:

$$
\left\{\begin{array}{l}
\Delta \Phi_{1}(r)-\kappa_{1}^{2} \Phi_{1}(r)=\frac{d^{2} \Phi_{1}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{1}(r)}{d r}-\kappa_{1}^{2} \Phi_{1}(r)=0 \\
\Delta \Phi_{2}(r)-\kappa_{2}^{2} \Phi_{2}(r)=\frac{d^{2} \Phi_{2}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{2}(r)}{d r}-\kappa_{2}^{2} \Phi_{2}(r)=-\kappa_{R}^{2} \Phi_{1}(r) \\
\quad \text { with }\left\{\begin{array}{l}
\kappa_{1}^{2} \equiv \frac{\Sigma_{a, 1}+\Sigma_{1 \rightarrow 2}}{D_{1}} \\
\kappa_{2}^{2} \equiv \frac{\Sigma_{a, 2}}{D_{2}} \\
\kappa_{R}^{2} \equiv \frac{\Sigma_{1 \rightarrow 2}}{D_{2}}
\end{array}\right.
\end{array}\right.
$$

and using the constant boundary conditions:

$$
\begin{cases}\Phi_{1}\left(R_{c}\right)=\Phi_{1}^{R_{c}} & \Phi_{1}\left(R_{R}\right)=\Phi_{1}^{R_{R}} \\ \Phi_{2}\left(R_{c}\right)=\Phi_{2}^{R_{c}} & \Phi_{2}\left(R_{R}\right)=\Phi_{2}^{R_{R}}\end{cases}
$$

The usual solution to the fast equation is given by the composition of zero-order Bessel functions:

$$
\Phi_{1}(r)=\Phi_{1}^{I} I_{0}\left(\kappa_{1} r\right)+\Phi_{1}^{K} K_{0}\left(\kappa_{1} r\right)
$$

The constant coefficients $\Phi_{1}^{I}$ and $\Phi_{1}^{K}$ are evaluated using the boundary conditions, thus leading to:

$$
\begin{aligned}
\Phi_{1}(r)= & \Phi_{1}^{R_{C}} \frac{I_{0}\left(\kappa_{1} r\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} r\right)}{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} R_{C}\right)} \\
& +\Phi_{1}^{R_{R}} \frac{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} r\right)-I_{0}\left(\kappa_{1} r\right) K_{0}\left(\kappa_{1} R_{C}\right)}{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} R_{C}\right)}
\end{aligned}
$$

The general solution to the thermal equation is obtained as the sum of the solution to the homogeneous equation (no LHS), and a particular solution of the inhomogeneous equation:

$$
\Phi_{2}(r)=\underbrace{\Phi_{2}^{I} I_{0}\left(\kappa_{2} r\right)+\Phi_{2}^{K} K_{0}\left(\kappa_{2} r\right)}_{\text {general solution without LHS }}+\underbrace{\frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}} \Phi_{1}(r)}_{\text {particular solution }}
$$

Once again, the boundary conditions are used to determine the constants $\Phi_{2}^{I}$ and $\Phi_{2}^{K}$ :

$$
\begin{aligned}
\Phi_{2}(r)= & \frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}} \Phi_{1}(r) \\
& +\left[\Phi_{2}^{R_{C}}-\frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}}\right]\left[\frac{I_{0}\left(\kappa_{2} r\right) K_{0}\left(\kappa_{2} R_{R}\right)-I_{0}\left(\kappa_{2} R_{R}\right) K_{0}\left(\kappa_{2} r\right)}{I_{0}\left(\kappa_{2} R_{C}\right) K_{0}\left(\kappa_{2} R_{R}\right)-I_{0}\left(\kappa_{2} R_{R}\right) K_{0}\left(\kappa_{2} R_{C}\right)}\right] \\
& +\left[\Phi_{2}^{R_{R}}-\frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}}\right]\left[\frac{I_{0}\left(\kappa_{2} R_{C}\right) K_{0}\left(\kappa_{2} r\right)-I_{0}\left(\kappa_{2} r\right) K_{0}\left(\kappa_{2} R_{C}\right)}{I_{0}\left(\kappa_{2} R_{C}\right) K_{0}\left(\kappa_{2} R_{R}\right)-I_{0}\left(\kappa_{2} R_{R}\right) K_{0}\left(\kappa_{2} R_{C}\right)}\right]
\end{aligned}
$$

The calculation of the net currents is employed to set up the $\mathfrak{R}$ matrix of the Poincaré-Steklov operator:

$$
\left\{\begin{aligned}
-D_{1} \frac{\partial \Phi_{1}(r)}{\partial r}=-D_{1} \kappa_{1}\left[\Phi_{1}^{R_{C}}\right. & \left.\frac{I_{1}\left(\kappa_{1} r\right) K_{0}\left(\kappa_{1} R_{R}\right)+I_{0}\left(\kappa_{1} R_{R}\right) K_{1}\left(\kappa_{1} r\right)}{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} R_{C}\right)}-\Phi_{1}^{R_{R}} \frac{I_{0}\left(\kappa_{1} R_{C}\right) K_{1}\left(\kappa_{1} r\right)+I_{1}\left(\kappa_{1} r\right) K_{0}\left(\kappa_{1} R_{C}\right)}{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} R_{C}\right)}\right] \\
-D_{2} \frac{\partial \Phi_{2}(r)}{\partial r}= & -D_{2} \frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}} \frac{\partial \Phi_{1}(r)}{\partial r}-D_{2} \kappa_{2}\left[\Phi_{2}^{R_{C}}-\frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}}\right]\left[\frac{I_{1}\left(\kappa_{2} r\right) K_{0}\left(\kappa_{2} R_{R}\right)+I_{0}\left(\kappa_{2} R_{R}\right) K_{1}\left(\kappa_{2} r\right)}{I_{0}\left(\kappa_{2} R_{C}\right) K_{0}\left(\kappa_{2} R_{R}\right)-I_{0}\left(\kappa_{2} R_{R}\right) K_{0}\left(\kappa_{2} R_{C}\right)}\right] \\
& +D_{2} \kappa_{2}\left[\Phi_{2}^{R_{R}}-\frac{\kappa_{R}^{2}}{\kappa_{2}^{2}-\kappa_{1}^{2}}\right]\left[\frac{I_{0}\left(\kappa_{2} R_{C} K_{1}\left(\kappa_{2} r\right)+I_{1}\left(\kappa_{2} r\right) K_{0}\left(\kappa_{2} R_{C}\right)\right.}{I_{0}\left(\kappa_{2} R_{C}\right) K_{0}\left(\kappa_{2} R_{R}\right)-I_{0}\left(\kappa_{2} R_{R}\right) K_{0}\left(\kappa_{2} R_{C}\right)}\right]
\end{aligned}\right.
$$

Poincaré-Steklov operator for a finite cylindrical reflector:

$$
\begin{align*}
J_{R_{C}, R_{R}} & =\left[\begin{array}{cc}
-D_{1} & \left(\frac{\partial \Phi_{1}}{\partial r}\right)_{R_{c}} \\
-D_{1} & \left(\frac{\partial \Phi_{1}}{\partial r}\right)_{R_{R}} \\
-D_{2}\left(\frac{\partial \Phi_{2}}{\partial r}\right)_{R_{c}} \\
-D_{2}\left(\frac{\partial \Phi_{2}}{\partial r}\right)_{R_{R}}
\end{array}\right] \\
& =\left[\begin{array}{cccc}
\mathfrak{R}_{11}^{C}\left(R_{C}\right) & \Re_{11}^{R}\left(R_{C}\right) & 0 & 0 \\
-\mathfrak{R}_{11}^{C}\left(R_{R}\right) & -\Re_{11}^{R}\left(R_{R}\right) & 0 & 0 \\
\mathfrak{R}_{12}^{R_{C}}\left(R_{c}\right) & \mathfrak{R}_{12}^{R_{R}}\left(R_{C}\right) & \mathfrak{R}_{22}^{R_{C}}\left(R_{c}\right) & \mathfrak{R}_{22}^{R_{R}}\left(R_{c}\right) \\
-\Re_{12}^{R_{C}}\left(R_{R}\right) & -\mathfrak{R}_{12}^{R_{R}}\left(R_{R}\right) & -\mathfrak{R}_{22}^{R_{C}}\left(R_{R}\right) & -\Re_{22}^{R_{R}}\left(R_{R}\right)
\end{array}\right]\left[\begin{array}{c}
\Phi_{1}^{R_{c}} \\
\Phi_{1}^{R_{R}} \\
\Phi_{2}^{R_{C}} \\
\Phi_{2}^{R_{R}}
\end{array}\right] \tag{13.10}
\end{align*}
$$

with (for the sake of brevity, only the first terms of the matrix are given; the others are readily obtained by identification):

$$
\left\{\begin{array}{l}
\mathfrak{R}_{11}^{C}(r)=-D_{1} \kappa_{1} \frac{I_{1}\left(\kappa_{1} r\right) K_{0}\left(\kappa_{1} R_{R}\right)+I_{0}\left(\kappa_{1} R_{R}\right) K_{1}\left(\kappa_{1} r\right)}{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} R_{C}\right)} \\
\mathfrak{R}_{11}^{R}(r)=+D_{1} \kappa_{1} \frac{I_{0}\left(\kappa_{1} R_{C}\right) K_{1}\left(\kappa_{1} r\right)+I_{1}\left(\kappa_{1} r\right) K_{0}\left(\kappa_{1} R_{C}\right)}{I_{0}\left(\kappa_{1} R_{C}\right) K_{0}\left(\kappa_{1} R_{R}\right)-I_{0}\left(\kappa_{1} R_{R}\right) K_{0}\left(\kappa_{1} R_{C}\right)}
\end{array}\right.
$$

### 13.2.4.3 Flux in Two Dimensions

Compared to the previous case, a more general case is obtained by considering a problem without radial symmetry:

$$
\left\{\begin{array}{l}
\Delta \Phi_{1}(r, \theta)-\kappa_{1}^{2} \Phi_{1}(r, \theta)=\frac{d^{2} \Phi_{1}(r, \theta)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{r 1}(r, \theta)}{d r}+\frac{1}{r^{2}} \frac{d^{2} \Phi_{r 1}(r, \theta)}{d \vartheta^{2}}-\kappa_{1}^{2} \Phi_{1}(r, \theta)=0 \\
\Delta \Phi_{2}(r, \theta)-\kappa_{2}^{2} \Phi_{2}(r, \theta)=\frac{d^{2} \Phi_{2}(r)}{d r^{2}}+\frac{1}{r} \frac{d \Phi_{2}(r, \theta)}{d r}+\frac{1}{r^{2}} \frac{d^{2} \Phi_{2}(r, \theta)}{d \vartheta^{2}}-\kappa_{2}^{2} \Phi_{2}(r, \theta)=-\kappa_{R}^{2} \Phi_{1}(r, \theta)
\end{array}\right.
$$

with the following boundary conditions:

$$
\begin{cases}\Phi_{1}\left(R_{c}, \theta\right)=\Phi_{1}^{R_{c}}(\theta) & \Phi_{1}\left(R_{R}, \theta\right)=\Phi_{1}^{R_{R}}(\theta) \\ \Phi_{2}\left(R_{c}, \theta\right)=\Phi_{2}^{R_{c}}(\theta) & \Phi_{2}\left(R_{R}, \theta\right)=\Phi_{2}^{R_{R}}(\theta)\end{cases}
$$

It is then assumed that the flux can be expanded as two functions that separate the variables $r$ and $\theta$ :

$$
\Phi_{g}(r, \theta)=\varphi_{g}(r) \phi_{g}(\theta)
$$

The usual method for dealing with this problem is to expand the angular flux in a Fourier series:

$$
\phi_{g}(\theta)=\sum_{n=0}^{\infty} \phi_{g, n}^{\mathrm{cos}} \cos n \theta+\phi_{g, n}^{\sin } \sin n \theta
$$

The general solution to the fast diffusion equation is thus obtained as:

$$
\begin{aligned}
\Phi_{g}(r, \theta)= & \sum_{n=0}^{\infty} \Phi_{g, n}^{\cos , I} \cos n \theta I_{n}\left(\kappa_{1} r\right)+\Phi_{g, n}^{\cos , K} \cos n \theta \quad K_{n}\left(\kappa_{1} r\right) \\
& +\Phi_{g, n}^{\sin , I} \sin n \theta I_{n}\left(\kappa_{1} r\right)+\Phi_{g, n}^{\sin , K} \sin n \theta \quad K_{n}\left(\kappa_{1} r\right)
\end{aligned}
$$

The boundary conditions can also be expanded into Fourier series:

$$
\left\{\begin{array} { l } 
{ \Phi _ { 1 } ( R _ { c } , \theta ) = \sum _ { n = 0 } ^ { \infty } \alpha _ { 1 } ^ { R _ { c } } \operatorname { c o s } n \theta + \beta _ { 1 } ^ { R _ { c } } \operatorname { s i n } n \theta } \\
{ \Phi _ { 2 } ( R _ { c } , \theta ) = \sum _ { n = 0 } ^ { \infty } \alpha _ { 2 } ^ { R _ { c } } \operatorname { c o s } n \theta + \beta _ { 2 } ^ { R _ { c } } \operatorname { s i n } n \theta }
\end{array} \left\{\begin{array}{l}
\Phi_{1}\left(R_{R}, \theta\right)=\sum_{n=0}^{\infty} \alpha_{1}^{R_{R}} \cos n \theta+\beta_{1}^{R_{R}} \sin n \theta \\
\Phi_{2}\left(R_{R}, \theta\right)=\sum_{n=0}^{\infty} \alpha_{2}^{R_{R}} \cos n \theta+\beta_{2}^{R_{R}} \sin n \theta
\end{array}\right.\right.
$$

The $\Phi_{g, n}^{\alpha}$ constants are determined by identification with the coefficients of $\cos n \theta$ or $\sin n \theta$ in the flux equation at the boundary conditions, assuming that these series converge. The same formulae as in the previous paragraph are hence obtained. The matrix of the Poincaré-Steklov operator is obtained as previously-using the net current that includes the derivatives of the $n t h$-order Bessel functions expressed using the recurrence relations for the derivatives. Using a fairly tedious identification process, the proportionality between the angular current and the angular flux at the interface may be established:

$$
J_{R_{C}, R_{R}}(\theta)=\left[\begin{array}{cccc}
\mathfrak{R}_{11}^{C}\left(R_{C}, \theta\right) & \mathfrak{R}_{11}^{R}\left(R_{C}, \theta\right) & 0 & 0 \\
-\mathfrak{R}_{11}^{C}\left(R_{R}, \theta\right) & -\mathfrak{R}_{11}^{R}\left(R_{R}, \theta\right) & 0 & 0 \\
\mathfrak{R}_{12}^{R_{C}}\left(R_{C}, \theta\right) & \mathfrak{R}_{12}^{R_{R}}\left(R_{C}, \theta\right) & \mathfrak{R}_{22}^{R_{C}}\left(R_{c}, \theta\right) & \mathfrak{R}_{22}^{R_{R}}\left(R_{c}, \theta\right) \\
-\mathfrak{R}_{12}^{R_{C}}\left(R_{R}, \theta\right) & -\mathfrak{R}_{12}^{R_{R}}\left(R_{R}, \theta\right) & -\mathfrak{R}_{22}^{R_{C}}\left(R_{R}, \theta\right) & -\mathfrak{R}_{22}^{R_{R}}\left(R_{R}, \theta\right)
\end{array}\right]\left[\begin{array}{c}
\Phi_{1}^{R_{c}}(\theta) \\
\Phi_{1}^{R_{R}}(\theta) \\
\Phi_{2}^{R_{C}}(\theta) \\
\Phi_{2}^{R_{R}}(\theta)
\end{array}\right]
$$

This expression is identical in all respects to the $1 D$ calculation, applied in each direction.

### 13.3 Definition of Reflector Albedo

In the case of a $P W R$, the fuel zone is surrounded by a reflector that is mostly composed of water (solid structures are also present, e.g. for the upper reflector of a $P W R$ : the non-inserted rods, the upper pin plugs, the steel structures of the upper plenum, etc.). For a fast reactor, the reflector is made up of steel structures and most probably of the coolant material. The extrapolation length is computed using the notion of albedo (the Latin word for "whiteness"), which characterizes the reflective properties of neutrons.

Let us consider two different media separated by a surface. The core fuel medium (c) situated on the left of the figure is multiplying, while the medium on the right of the figure is the reflector $(r)$. Neutrons exit the fuel medium and some return to the core zone after one or more collisions in the reflector. In the case of a physical reflector, some neutrons are absorbed and will not be reflected back to the core. The incoming current in the fuel is thus logically lower than the outgoing current (Fig. 13.7).

The albedo $\beta$ of a reflector is the ratio of the outgoing current from the reflector ( $J_{r}^{-}$(black) moving from $r \rightarrow c$ ), i.e. returning to the core zone) to the incoming current in the reflector ( $J_{r}^{+}$(grey) moving from $c \rightarrow r$ ), i.e. leaving the fuel medium). It should be noted that the reciprocal of the situation depicted in the figure would define the fuel albedo as the ratio of the outgoing current from the core to the

Fig. 13.7 Fuel medium reflected by a reflective medium

incoming current in the core. The reflector albedo and the fuel albedo are thus intrinsically related since:

$$
J_{r}^{-}=J_{c}^{+} \quad \text { and } \quad J_{r}^{+}=J_{c}^{-}
$$

In diffusion theory and in one dimension using $x$ to simplify the notations, the reflector albedo $\beta$ is defined by the formula (with $\Phi_{0}$ being the flux at the interface):

$$
\beta=\frac{J_{r}^{-}}{J_{r}^{+}}=\frac{\frac{\Phi_{0}}{4}+\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{r}}{\frac{\Phi_{0}}{4}-\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{r}}=\frac{J_{c}^{+}}{J_{c}^{-}}=\frac{\frac{\Phi_{0}}{4}+\frac{D_{c}}{2}\left(\frac{d \Phi}{d x}\right)_{c}}{\frac{\Phi_{0}}{4}-\frac{D_{c}}{2}\left(\frac{d \Phi}{d x}\right)_{c}}
$$

The albedo $\beta$ characterizes the reflector medium when written as:

$$
\beta=J_{r}^{-} / J_{r}^{+}=\left(\frac{\Phi_{0}}{4}+\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{r}\right) /\left(\frac{\Phi_{0}}{4}-\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{r}\right)
$$

but it can also characterize the fuel medium if written as:

$$
\beta=J_{c}^{+} / J_{c}^{-}=\left(\frac{\Phi_{0}}{4}+\frac{D_{c}}{2}\left(\frac{d \Phi}{d x}\right)_{c}\right) /\left(\frac{\Phi_{0}}{4}-\frac{D_{c}}{2}\left(\frac{d \Phi}{d x}\right)_{c}\right)
$$

The fuel medium becomes in some respects the "reflector" for the reflector medium. It should be noted that since $(d \Phi / d x)_{r}<0, \beta$ is lower than 1 and tends towards 1 as $(d \Phi / d x)_{r}$ tends towards 0 (corresponding to a flat flux), this is in fact a case of "mirror" reflection:

$$
\begin{equation*}
\text { Mirror reflection: } \quad J_{r}^{-}=J_{r}^{+}=J_{c}^{-}=J_{c}^{+}=\frac{\Phi_{0}}{4} \tag{13.11}
\end{equation*}
$$

Similarly, for the net current:

$$
J_{c}^{n e t}=-D_{c} \operatorname{grad} \Phi_{c}=J_{c}^{-}-J_{c}^{+}=0
$$

In the general case of a reflection by an albedo different from 1, the derivative of the flux in the reflector depends only on $\Phi_{0}, \beta$ and $D_{r}$ (Etherington 1957, pp. 6-18):

$$
\frac{\left(\frac{d \Phi}{d x}\right)_{r}}{\Phi_{0}}=-\frac{1}{2 D_{r}} \frac{1-\beta}{1+\beta}
$$

Similarly, on the fuel side:

Logarithmic derivative of the flux at the interface:

$$
\begin{equation*}
\frac{\left(\frac{d \Phi}{d x}\right)_{c}}{\Phi_{0}}=-\frac{1}{2 D_{c}} \frac{1-\beta}{1+\beta} \tag{13.12}
\end{equation*}
$$

This relation allows substitution of a calculation with two media by a diffusion calculation on the first medium only, with boundary conditions set on the logarithmic derivative of the flux, without computation of the flux in the reflector. This type of boundary condition is called an albedo condition. In practice, using this method, the calculation mesh has fewer cells since there is no need to mesh the reflector, and thus, a gain in computation time results.

### 13.3.1 Albedo Calculation for a Slab Reflector

When neutrons are injected from any source, the thermal flux in the infinite reflector is given by the classical attenuation formula:

$$
\Phi(x)=\Phi(0) e^{-\frac{x}{L}}
$$

The thermal neutron flux level at the origin $\Phi(0)$ depends on the neutron source. The reflector albedo is calculated by:

$$
\begin{equation*}
\text { Albedo of a slab reflector: } \quad \beta=\frac{\left(\frac{\Phi_{0}}{4}+\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{0}\right)}{\left(\frac{\Phi_{0}}{4}-\frac{D_{r}}{2} \quad\left(\frac{d \Phi}{d x}\right)_{0}\right)}=\frac{1-2 \frac{D_{r}}{L_{r}}}{1+2 \frac{D_{r}}{L_{r}}} \tag{13.13}
\end{equation*}
$$

It can be seen that it does not depend on the initial flux level, thus the source. The reflector tends towards a mirror when $D_{r} / L_{r}$ tends towards 0 (Fig. 13.8).

For a reflector of finite thickness $a$, the flux in the reflector that turns zero at a distance $a+\delta$ is written as:

Fig. 13.8 Infinite slab reflector


$$
\Phi(x)=\Phi(0) \frac{\operatorname{sh}(a+\delta-x)}{\operatorname{sh}(a+\delta)}
$$

A calculation analogous to the previous one but with this new flux shape leads to:

$$
\beta=\frac{1-2 \frac{D_{r}}{L_{r}} \operatorname{coth}\left(\frac{a+\delta}{L_{r}}\right)}{1+2 \frac{D_{r}}{L_{r}} \operatorname{coth}\left(\frac{a+\delta}{L_{r}}\right)}
$$

### 13.3.2 Albedo Calculation of a Cylindrical Reflector

In the case of a cylindrical reflector surrounding a cylindrical source of radius $R$, the flux in the reflector is given by:

$$
\Phi(r \geq R)=\Phi(0) \frac{K_{0}\left(r / L_{r}\right)}{K_{0}\left(R / L_{r}\right)}
$$

and the albedo for the cylindrical reflector is written as:
Albedo of a cylindrical reflector:

$$
\begin{equation*}
\left.\beta=\frac{\left(\frac{\Phi_{0}}{4}+\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{0}\right)}{\left(\frac{\Phi_{0}}{4}-\frac{D_{r}}{2}\right.}\left(\frac{d \Phi}{d x}\right)_{0}\right) \quad=\frac{1-2 \frac{D_{r}}{L_{r} K_{0}\left(R / L_{r}\right)} K_{1}\left(R / L_{r}\right)}{1+2 \frac{D_{r}}{L_{r} K_{0}\left(R / L_{r}\right)} K_{1}\left(R / L_{r}\right)} \tag{13.14}
\end{equation*}
$$

### 13.3.3 Albedo of a Spherical Reflector

In the case of spherical reflector surrounding a spherical source of radius $R$, the flux in the reflector is given by:

$$
\Phi(r \geq R)=\Phi(0) \frac{R}{r} e^{-\frac{r-R}{L r}}
$$

As previously, the albedo is computed as:

Albedo of a spherical reflector:

$$
\begin{equation*}
\left.\beta=\frac{\left(\frac{\Phi_{R}}{4}+\frac{D_{r}}{2}\left(\frac{d \Phi}{d r}\right)_{R}\right)}{\left(\frac{\Phi_{R}}{4}-\frac{D_{r}}{2}\right.}\left(\frac{d \Phi}{d x}\right)_{R}\right) \quad=\frac{1-2 D_{r}\left(\frac{1}{L_{r}}+\frac{1}{R}\right)}{1+2 D_{r}\left(\frac{1}{L_{r}}+\frac{1}{R}\right)} \tag{13.15}
\end{equation*}
$$

### 13.3.4 Albedo Calculation for the Upper Reflector of a Cylindrical Reactor

The flux in an axially-finite cylindrical reactor was illustrated earlier. This flux solution is extrapolated in the upper reflector, as expressed earlier in the theory assuming an infinite reflector. This result is an approximation since the flux in a finite cylinder surrounded by a reflector cannot be expressed as functions of the radius and the height separately. However, in the fuel, it may be hypothesized that $\Phi(r, z) \approx \Phi_{\max } J_{0}\left(j_{0,1} r / R\right) \cos (\pi z / H)$. In practical cases, the value of $H$ is equal to the active height of the core added to twice $\delta$ for which the cosine of the flux cancels out: $H=H_{\text {act }}+2 \delta$. This distance at which the flux is zero is often confused with extrapolation distance $d$ given in diffusion theory for a bare reactor (surrounded by a vacuum) by the formula (see the chapter on the Boltzmann equation and the Milne problem): $d=0.7104 \lambda_{\text {transport }}$. This extrapolation distance is the point at which the derivative of the flux from the fuel zone crosses the $z$-axis. The transport length $\lambda_{\text {transport }}=3 D_{c}$ is given by $D_{c}$, where $D_{c}$ is the fuel diffusion coefficient.

Let us consider the flux in the axial reflector. Strictly speaking, the extrapolation distance does not correspond to the distance at which the cosine of the flux is equal to zero, but diverges from this value as the flux at $a / 2$ approaches the maximum flux at 0 . This value for the flux in the fuel is then extrapolated in the reflector by multiplying it by a decreasing exponential, as illustrated in the calculations for the reflector in slab geometry accounting for a shift in the $z$-axis. In the radial reflector, the exact flux solution involves the Bessel function $K_{0}$. However, in the radial direction, close to the interface with the reactor, it has been shown that a simpler expression may be employed with a decreasing exponential applied to the fuel flux at the interface. Hence, in the axial reflector, the solution is not separable and impacts the flux solution in the radial reflector as it approaches the radius of the cylinder. The boundary effects are not considered for the time being so as to simplify the problem, thereby leading to the solution:

$$
\left\{\begin{array}{l}
\Phi(r, z) \approx \Phi_{\max } J_{0}\left(j_{0,1} \frac{r}{R}\right) \cos \left(\pi \frac{H_{a c t}}{2 H}\right) e^{-\kappa_{r}\left(z-\frac{H_{a c t}^{2}}{2}\right)} \quad \text { with } \quad \kappa_{r}^{2}=\frac{\Sigma_{a}^{r}}{D_{r}}=\frac{1}{L_{r}^{2}} \\
J\left(r, \frac{H_{a c t}}{2}\right)=-D_{r} \operatorname{grad}\left(\Phi_{r}(r, z)\right)_{\frac{H_{a c t}}{2}}=D_{r} \kappa_{r} \Phi_{\frac{H_{a c t}}{2}}=\frac{D_{r}}{L_{r}} \Phi_{\frac{H_{a c t}}{2}}
\end{array}\right.
$$

By definition of the extrapolation distance $d$, on the fuel side we have:

$$
\Phi_{\frac{H_{a c t}}{2}}+d \operatorname{grad}\left(\Phi_{c}(r, z)\right)_{\frac{H_{a c t}}{2}}=0
$$

 definition of the albedo:

$$
\beta=\frac{J_{r}^{-}}{J_{r}^{+}}=\left(\frac{\Phi_{\frac{H_{a c t}}{2}}}{4}+\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{r, \frac{H_{a c t}}{2}}\right) /\left(\frac{\Phi_{\frac{H_{a c c}}{2}}}{4}-\frac{D_{r}}{2}\left(\frac{d \Phi}{d x}\right)_{r, \frac{H_{a c t}}{2}}\right)
$$

The current at the core/reflector interface is substituted by the following expression:

$$
D_{r}\left(\frac{d \Phi}{d x}\right)_{r, \frac{H_{a c t}}{2}}=-J_{\frac{H_{\text {act }}}{2}}=-\Phi_{\frac{H_{a c t}}{2}} \frac{D_{r}}{L_{r}}
$$

Thus, the reflector albedo in diffusion is written as:
Albedo as a function of the reflector properties:

$$
\begin{equation*}
\beta=\frac{1-2 D_{r} / L_{r}}{1+2 D_{r} / L_{r}}=\frac{1-2 D_{c} / d}{1+2 D_{c} / d} \tag{13.16}
\end{equation*}
$$

### 13.3.5 Extrapolation and Null-flux Distances

The null-flux distance for the flux $\delta$ (Fig. 13.9) is the length added to the active height (in reality, twice this distance: $H=H_{a c t}+2 \delta$ ) to extrapolate the cosine in $z$. It is often confused with the extrapolation distance $d$ but has a different value, especially if the reactor is small.
$\delta$ can be expressed as a function of the albedo for a large cylindrical reactor seen with $P W R$ : the previous formula for the theoretical flux, presented in the last section, is applied:

Fig. 13.9 Difference between the extrapolation distance $d$ and the null-flux distance of cosine $\delta$


$$
\left.\frac{\partial \Phi(r, x)}{\partial z}\right|_{c}=\Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R} r\right)\left[-\frac{\pi}{H} \sin \left(\frac{\pi z}{H}\right)\right]_{\frac{H_{a c t}}{2}}
$$

thus:

$$
\frac{\left.\frac{d \Phi}{d z}\right|_{c}}{\Phi_{0}}=\frac{\Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R} r\right)\left[-\frac{\pi}{H} \sin \left(\frac{\pi z}{H}\right)\right]_{\frac{H_{\text {act }}}{2}}}{\Phi_{\max } J_{0}\left(\frac{j_{0,1}}{R} r\right)\left[\cos \left(\frac{\pi z}{H}\right)\right]_{\frac{H_{\text {act }}}{2}}}=-\frac{1}{2 D_{c}} \frac{1-\beta}{1+\beta}
$$

Finally:

$$
\frac{\pi}{H} \tan \left(\frac{\pi}{2} \frac{H_{\text {act }}}{H}\right)=\frac{1}{2 D_{c}} \frac{1-\beta}{1+\beta}
$$

Assuming that the null-flux distance is small compared to $H_{\text {act }}=H-2 \delta$ :

$$
\tan \left(\frac{\pi}{2} \frac{H_{a c t}}{H}\right) \approx \tan \left(\frac{\pi}{2}\left(1-\frac{2 \delta}{H_{a c t}}\right)\right)=\cot \left(\frac{2 \delta}{H_{a c t}}\right)
$$

Since $\cot (x)=\frac{1}{x}-\frac{x}{3}-\ldots$ when $x^{2}<\pi^{2}$, it may be inferred that:

$$
\frac{\pi}{H} \cot \left(\frac{2 \delta}{H_{a c t}}\right) \approx \frac{\pi}{\left(H_{a c t}+2 \delta\right)}\left[\frac{H_{a c t}}{2 \delta}-\frac{2 \delta}{3 H_{a c t}}\right]=\frac{1}{2 D_{c}} \frac{1-\beta}{1+\beta}
$$

Expanding $\frac{1}{\left(1+\frac{2 \delta}{H_{a c t}}\right)} \approx\left(1-\frac{2 \delta}{H_{\text {act }}}+\left(\frac{2 \delta}{H_{\text {act }}}\right)^{2}\right)$ into Taylor series leads to:

$$
\frac{\pi}{H_{a c t}}\left(\frac{H_{\text {act }}}{2 \delta}-1-\frac{2 \delta}{3 H_{\text {act }}}+\frac{2 \delta}{H_{\text {act }}}+\frac{4 \delta^{2}}{3 H_{\text {act }}{ }^{2}}+\ldots\right)=\frac{1}{2 D_{c}} \frac{1-\beta}{1+\beta}
$$

which, at first order, is:

Null-flux distance expressed in terms of albedo:

$$
\begin{equation*}
\delta \approx \pi D_{c} \frac{1+\beta}{1-\beta} \tag{13.17}
\end{equation*}
$$

This approximated analytical solution leads to the calculation of $\delta$ where the diffusion coefficient in the core and the albedo of the upper or lower reflector are known. Using an albedo $\beta$ of 0.8 for water at $20^{\circ} \mathrm{C}$ and a fuel diffusion coefficient of $1.3236 \mathrm{~cm}, \delta$ is 37.4 cm , i.e. approximately 40 cm as an order of magnitude.

Similarly, the extrapolation distance $d$ is calculated in terms of the null-flux distance $\delta$ as follows. The equation for the tangent to the flux that crosses the $z$-axis at the extrapolation distance is given by:

$$
\Phi(z)=\left(\frac{d \Phi}{d z}\right)_{\frac{H_{a c t}}{2}}\left(z-\frac{H_{a c t}}{2}\right)+\Phi_{0}
$$

This line crosses the $z$-axis at the position $z_{d}$, thus:

$$
\begin{aligned}
d & =\frac{H}{\pi} \tan \left(\frac{2 \delta}{H_{a c t}}\right)=\frac{\left(H_{a c t}+2 \delta\right)}{\pi}\left(\frac{2 \delta}{H_{a c t}}+\frac{8 \delta^{3}}{3 H_{a c t}^{3}}+\ldots\right) \\
& =\frac{2 \delta}{\pi}+\frac{4 \delta^{2}}{\pi H_{a c t}}+\frac{8 \delta^{3}}{3 \pi H_{a c t}{ }^{2}}+\frac{16 \delta^{4}}{3 \pi H_{a c t}{ }^{3}}+\ldots
\end{aligned}
$$

using the calculation results given previously for the null-flux distance. The extrapolation distance $d$ is expressed as $d=z_{d}-H_{\text {act }} / 2$. Using the Taylor expansion of $\tan (x)$ in the neighborhood of $0: \tan (x)=x+x^{3} / 3+\ldots$, we obtain:

$$
\begin{aligned}
d & =\frac{H}{\pi} \tan \left(\frac{2 \delta}{H_{a c t}}\right)=\frac{\left(H_{a c t}+2 \delta\right)}{\pi}\left(\frac{2 \delta}{H_{a c t}}+\frac{8 \delta^{3}}{3 H_{a c t}^{3}}+\ldots\right) \\
& =\frac{2 \delta}{\pi}+\frac{4 \delta^{2}}{\pi H_{a c t}}+\frac{8 \delta^{3}}{3 \pi H_{a c t}{ }^{2}}+\frac{16 \delta^{4}}{3 \pi H_{a c t}{ }^{3}}+\ldots
\end{aligned}
$$

Finally, the extrapolation distance $d$ is given in terms of the null-flux distance $\delta$ by:

Extrapolation distance in terms of the null-flux distance:

$$
\begin{equation*}
d=\frac{2 \delta}{\pi}+\frac{4 \delta^{2}}{\pi H_{a c t}}+\frac{8 \delta^{3}}{3 \pi H_{a c t}{ }^{2}}+\frac{16 \delta^{4}}{3 \pi H_{a c t}{ }^{3}}+\ldots \tag{13.18}
\end{equation*}
$$

It should be noted that this expression for the extrapolation distance must not be simplified to the first term only, since this would imply that it is smaller than nullflux distance (as $2 \delta / \pi<\delta$ ). However, it is clear that the extrapolation distance $d$ is

Table 13.1 Albedos of some usual reflectors

|  | Density $\mathrm{g} \cdot$ <br> $\mathrm{cm}^{-3}$ | 1.1 | $\lambda_{t r}=3 \mathrm{D} \mathrm{cm}$ | D cm |
| :--- | :--- | :--- | :--- | :--- |$\beta_{[-]}$.

larger than the null-flux distance $\delta$ (from the properties of the cosine function and its derivative between 0 and $\pi / 2$ ).

### 13.3.6 Numerical Example

The values of the diffusion coefficients and albedos for the main industrial moderators are given in Table 13.1. For the upper reflector of a 900 MWe light water reactor, the diffusion coefficient is computed using the formula $D=1 /\left(\begin{array}{ll}3 & \Sigma_{t r}\end{array}\right)$ where the macroscopic cross sections are obtained from a fuel/upper reflector slab calculation using the French code APOLLO2. Similarly, since $\Sigma_{\text {trreflector }}=0.36825 \mathrm{~cm}^{-1}$ and $\Sigma_{\text {absorption }}^{\text {reflect }}=0.0063333 \mathrm{~cm}^{-1}, D_{r}=0.905 \mathrm{~cm}$ and $L_{r}=11.95 \mathrm{~cm}$. Using $\beta=\left(1-2 D_{r} / L_{r}\right) /\left(1+2 D_{r} / L_{r}\right), \beta=0.737$ for the water+steel reflector of 900 MWe light water reactor. Since $\Sigma_{t r}^{\text {fuel }}=0.49243 \quad \mathrm{~cm}^{-1}$ and $\Sigma_{\text {absorption }}^{\text {fuel }}=0.03393 \mathrm{~cm}^{-1}$ for a $P W R$ fuel at $3.7 \%$ enrichment, $D_{c}=0.677 \mathrm{~cm}$ and $L_{c}=4.467 \mathrm{~cm}$, i.e. an albedo of 0.535 that is logically smaller than the values obtained for water only or for a true water+steel reflector of a $P W R$, given that fuel is strongly absorbing. The closer the albedo to 1 , the flatter the flux shape will be at the interface. An albedo of 1 represents the case of a mirror-like reflector, i.e. an infinite medium situation.

### 13.4 Reflector Theory with Two Energy Groups

If the reflector is analyzed in detail, it may be observed that a mono-energy theory is not satisfactory from an industrial viewpoint. In fact, the reflector modifies the flux spectrum at the core/reflector interface, which cannot be accounted for in one-group equations. This modification of the spectrum leads to significant variations of
several physical quantities. This is why the two-energy group calculations highlight a reflector effect that occur for all reflectors, but more particularly in $P W R$ : the thermal flux increases in the reflector since fast neutrons are quickly thermalized.

### 13.4.1 Slab Reflector

For slab geometries, the two-energy group flux equations in the reflector are written as:

$$
\begin{gathered}
\left\{\begin{array}{c}
-D_{1 r} \Delta \Phi_{1 r}(x)+\Sigma_{1, r} \Phi_{1 r}(x)=0 \\
-D_{2 r}
\end{array} \Delta \Phi_{2 r}(x)+\Sigma_{a 2, r} \Phi_{2 r}(x)=\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(x)\right. \\
\text { with }\left\{\begin{array}{c}
\Sigma_{1, r} \equiv \Sigma_{a_{1 r}}+\Sigma_{1 \rightarrow 2, r} \quad L_{1 r}^{2} \equiv \frac{D_{1 r}}{\Sigma_{1, r}} \\
L_{2 r}^{2} \equiv \frac{D_{2 r}}{\Sigma_{a 2, r}}
\end{array}\right.
\end{gathered}
$$

the solution of which in plane geometry, which is null at infinity, is given by:

$$
\left\{\begin{array}{c}
\Phi_{1 r}(x)=\Phi_{1 r}(0) e^{-\frac{x}{L_{1 r}}} \\
\Phi_{2 r}(x)=\alpha e^{-\frac{x}{L_{1 r}}}+\beta e^{-\frac{x}{L_{2 r}}}
\end{array}\right.
$$

The coefficients $\alpha$ and $\beta$ satisfy the system of equations below, by substituting the expressions of $\Phi_{2 r}(x)$ and $\Phi_{1 r}(x)$ in the differential equation for the thermal group:

$$
\left\{\begin{array}{c}
\alpha+\beta=\Phi_{2 r}(0) \\
\left(-\frac{D_{2 r}}{L_{1 r}^{2}}+\Sigma_{a 2, r}\right) \alpha=\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(0)
\end{array}\right.
$$

Leading to:
Fast and thermal flux in a slab reflector:

$$
\left\{\begin{array}{c}
\Phi_{1 r}(x)=\Phi_{1 r}(0) e^{-\frac{x}{L_{1 r}}}  \tag{13.19}\\
\Phi_{2 r}(x)=\Phi_{1 r}(0) \frac{\Sigma_{1 \rightarrow 2, r} L_{1 r}^{2}}{\left(\Sigma_{a 2, r} L_{1 r}^{2}-D_{2 r}\right)} e^{-\frac{x}{L_{1 r}}}+\left[\Phi_{2 r}(0)-\Phi_{1 r}(0) \frac{\Sigma_{R r} L_{1 r}^{2}}{\left(\Sigma_{a 2,2} L_{1 r}^{2}-D_{2 r}\right)}\right] e^{-\frac{x}{L_{2 r}}}
\end{array}\right.
$$

Analysis of the exponential terms for the thermal flux shows that if $L_{2 r}>L_{1 r}$, thermal neutrons may scatter far away while the fast component of the spectrum decays quickly, leading to a thermal spectrum, or even a Maxwell spectrum. This is the case for $U N G G$ reactors with graphite or heavy water. Otherwise ( $L_{2 r}<L_{1 r}$ ),
fast neutrons may travel deep into the reflector and the flux decays exponentially, while nevertheless maintaining its spectrum to a significant depth. This is the case of pure light water that attenuates the whole spectrum proportionally over a distance of 100 cm . For an industrial $P W R$ reflector containing thermal absorbers (boron, steel structures), an exponential decay of the fast flux is observed due to absorption, and mainly to scattering down the thermal group. Furthermore, an increase in the thermal flux is observed at around 40 cm owing to the weak absorption of water in the reflector compared to that in the fuel in the core. This increase is even greater if less boron is present in the water.

### 13.4.2 Infinite Cylindrical Reactor with Reflector in Two Groups Without Up-Scattering

Let us consider the cylindrical reactor previously illustrated in one energy group. The two-group diffusion equations without up-scattering for the core are expressed as:
(fast group 1)
$-D_{1 c} \Delta \Phi_{1 c}(r)+\Sigma_{1, c} \Phi_{1 c}(r)=\nu \Sigma_{f_{1 c}} \Phi_{1 c}(r)+\nu \Sigma_{f_{2 c}} \Phi_{2 c}(r)$
written in the following form by neglecting neutron production by the fast flux $\left(\nu \Sigma_{f_{1 c}} \Phi_{1 c}(r) \ll \nu \Sigma_{f_{2 c}} \Phi_{2 c}(r)\right)$ :

$$
\Delta \Phi_{1 c}(r)+B_{1 c}^{2} \Phi_{1 c}(r)=-\frac{\nu \Sigma_{f_{2 c}} \Phi_{2 c}(r)}{D_{1 c}}=-B_{f c}^{2} \Phi_{2 c}(r)
$$

with $B_{1 c}^{2}=\frac{\nu \Sigma_{f_{1 c}}-\Sigma_{1, c}}{D_{1 c}}=\frac{k_{x, c}-1}{L_{1 c}^{2}}$ and $B_{f c}^{2}=\frac{\nu \Sigma_{f_{c c}}}{D_{1 c}}$
(thermal group 2)

$$
-D_{2 c} \Delta \Phi_{2 c}(r)+\Sigma_{a 2, c} \Phi_{2 c}(r)=\Sigma_{1 \rightarrow 2, c} \Phi_{1 c}(r)
$$

written as:

$$
\Delta \Phi_{2 c}(r)-\kappa_{2 c}^{2} \Phi_{2 c}(r)=-\frac{\Sigma_{1 \rightarrow 2, c}}{D_{2 c}} \Phi_{1 c}(r)=-\kappa_{R c}^{2} \Phi_{1 c}(r)
$$

with $\kappa_{2 c}^{2}=\Sigma_{a 2, c} / D_{2 c}$ et $\kappa_{R c}^{2}=\Sigma_{1 \rightarrow 2, c} / D_{2 c}$
There is no fission source in the reflector:
(fast group 1) $-D_{1 r} \Delta \Phi_{1 r}(r)+\Sigma_{1, r} \Phi_{1 r}(r)=0$
expressed as:

$$
\Delta \Phi_{1 r}(r)-\kappa_{1 r}^{2} \Phi_{1 r}(r)=0 \quad \text { with } \quad \kappa_{1 r}^{2}=\Sigma_{1, r} / D_{1 r}
$$

(thermal group 2) $-D_{2 r} \Delta \Phi_{2 r}(r)+\Sigma_{a 2, r} \Phi_{2 r}(r)=\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(r)$
expressed as:

$$
\Delta \Phi_{2 r}(r)-\kappa_{2 r}^{2} \Phi_{2 r}(r)=-\frac{\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(r)}{D_{2 r}}=-\kappa_{R r}^{2} \Phi_{1 r}(r)
$$

with $\kappa_{2 r}^{2}=\Sigma_{a 2, r} / D_{2 r}$ and $\kappa_{R r}^{2}=\Sigma_{1 \rightarrow 2, r} / D_{2 r}$.

### 13.4.3 Flux Calculation in the Fuel

From the thermal equation for the fuel, we obtain: $\Phi_{1 c}(r)=-\frac{1}{\kappa_{R c}^{2}} \Delta \Phi_{2 c}(r)+\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}} \Phi_{2 c}(r)$ which is inserted in the fast equation for the fuel: Equation for thermal flux:

$$
\begin{align*}
& \Delta\left(-\frac{1}{\kappa_{R c}^{2}} \Delta \Phi_{2 c}(r)+\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}} \Phi_{2 c}(r)\right)+B_{1 c}^{2}\left(-\frac{1}{\kappa_{R c}^{2}} \Delta \Phi_{2 c}(r)+\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}} \Phi_{2 c}(r)\right) \\
&=-B_{f c}^{2} \Phi_{2 c}(r)-\frac{1}{\kappa_{R c}^{2}} \Delta \Delta \Phi_{2 c}(r)+\left(\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}}-\frac{B_{1 c}^{2}}{\kappa_{R c}^{2}}\right) \Delta \Phi_{2 c}(r) \\
&+B_{1 c}^{2}\left(\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}}+\frac{B_{f c}^{2}}{B_{1 c}^{2}}\right) \Phi_{2 c}(r)=0 \tag{13.20}
\end{align*}
$$

This equation, which contains only partial derivatives of order 2 and 4 , may be solved analytically by setting an intermediate function $F_{2 c}(r)=\Delta \Phi_{2 c}(r)-\lambda^{2} \Phi_{2 c}(r)$ that satisfies the following differential equation:

$$
\Delta F_{2 c}(r)+\mu^{2} F_{2 c}(r)=0
$$

or: $\Delta \Phi_{2 c}(r)+\left(\mu^{2}-\lambda^{2}\right) \Delta \Phi_{2 c}(r)-\mu^{2} \lambda^{2} \Phi_{2 c}(r)=0$
Identifying the coefficients of the previous equation with the physical equation gives:

$$
\left(\mu^{2}-\lambda^{2}\right)=B_{1 c}^{2}-\kappa_{2 c}^{2} \quad \text { and } \quad \mu^{2} \lambda^{2}=B_{1 c}^{2} \kappa_{R c}^{2}+B_{1 c}^{2} B_{f c}^{2}
$$

In this system of equation, $\lambda$ and $\mu$ can be easily determined analytically. The general solution to the equation $\Delta F_{2 c}(r)+\mu^{2} F_{2 c}(r)=0$ is of the form $F_{2 c}(r)=$ $A J_{0}(\mu r)+C Y_{0}(\mu r)$. The general solution to $\Delta \Phi_{2 c}(r)-\lambda^{2} \Phi_{2 c}(r)=0$ is of the form $\Phi_{2 c}(r)=G I_{0}(\lambda r)+H K_{0}(\lambda r)$. Hence, the general solution to the equation $\Delta \Phi_{2 c}(r)-\lambda^{2} \Phi_{2 c}(r)=F_{2 c}(r)$ can be expressed as:

$$
\Phi_{2 c}(r)=\Phi_{2 c}^{J} J_{0}(\mu r)+\Phi_{2 c}^{Y} Y_{0}(\mu r)+\Phi_{2 c}^{I} I_{0}(\lambda r)+\Phi_{2 c}^{K} K_{0}(\lambda r)
$$

Since the thermal flux in the fuel and the current are finite at $r=0$, the singular terms can be cancelled, i.e. $\Phi_{2 c}^{Y} Y_{0}(\mu r)$ and $\Phi_{2 c}^{K} K_{0}(\lambda r)$, thus $\Phi_{2 c}^{Y}=0$ and $\Phi_{2 c}^{K}=0$.

$$
\Phi_{2 c}(r)=\Phi_{2 c}^{J} J_{0}(\mu r)+\Phi_{2 c}^{I} I_{0}(\lambda r)
$$

Finally, we express that the flux is maximum at the center of the geometry: $\Phi_{2 c}(0)=\Phi_{2 c}^{J} \underbrace{J_{0}(0)}_{1}+\Phi_{2 c}^{I} \underbrace{I_{0}(0)}_{1}=\Phi_{2 c}^{J}+\Phi_{2 c}^{I}=\Phi_{2}^{c} \max$ and that, by symmetry, the current is zero at the center:

$$
-D_{2}^{c} \operatorname{grad} \Phi_{2 c}(r)=-D_{2 c}(-\Phi_{2 c}^{J} \mu \underbrace{J_{1}(0)}_{0}+\Phi_{2 c}^{I} \lambda \underbrace{I_{1}(0)}_{0})=0
$$

It is observed that, contrary to the one-group flux calculated for a bare or reflected reactor $\Phi(r)=\Phi_{\max } J_{0}\left(j_{0,1} r / R\right)$, the term $I_{0}(\lambda r)$, which increases with $r$, induces a rise in the thermal flux, illustrating the fact that the decrease in the fast flux is the source of thermal neutrons. The fast flux in the fuel is obtained as:

$$
\begin{aligned}
& \Phi_{1 c}(r)=-\frac{1}{\kappa_{R c}^{2}} \Delta \Phi_{2 c}(r)+\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}} \Phi_{2 c}(r)=-\frac{1}{\kappa_{R c}^{2}} \frac{1}{r} \frac{d}{d r}\left(r \frac{d \Phi_{2 c}(r)}{d r}\right)+\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}} \Phi_{2 c}(r) \\
& \Phi_{1 c}(r)= \\
& -\frac{1}{\kappa_{R c}^{2}}\left[\begin{array}{l}
\left.\left(-\Phi_{2 c}^{J} \mu^{2}\left(-\frac{1}{\mu r} J_{1}(\mu r)+J_{0}(\mu r)\right)+\Phi_{2 c}^{I} \lambda^{2}\left(-\frac{1}{\lambda r} I_{1}(\lambda r)+I_{0}(\lambda r)\right)\right)\right] \\
+\frac{1}{r}\left(-\Phi_{2 c}^{J} \mu J_{1}(\mu r)+\Phi_{2 c}^{I} \lambda I_{1}(\lambda r)\right) \\
+\frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}}\left(\Phi_{2 c}^{J} J_{0}(\mu r)+\Phi_{2 c}^{I} I_{0}(\lambda r)\right)
\end{array}\right.
\end{aligned}
$$

Hence: $\Phi_{1 c}(r)=\Phi_{2 c}^{J} \frac{\kappa_{c c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} J_{0}(\mu r)+\Phi_{2 c}^{I} \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}} I_{0}(\lambda r)$

As for the thermal flux, the following equations are obtained:

$$
\begin{aligned}
\Phi_{1 c}(0) & =\Phi_{2 c}^{J} \frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} J_{0}(0)+\Phi_{2 c}^{I} \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}} I_{0}(0) \\
& =\Phi_{2 c}^{J} \frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}}+\Phi_{2 c}^{I} \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}}=\Phi_{1 \mathrm{max}}
\end{aligned}
$$

This equation is coupled to that obtained for the thermal flux $\Phi_{2 c}^{J}+\Phi_{2 c}^{I}=\Phi_{2 c \text { max }}$ and enables evaluation of the constants $\Phi_{2 c}^{J}$ and $\Phi_{2 c}^{I}$ in terms of $\Phi_{1 c \text { max }}$ and $\Phi_{2 c \text { max }}$ using Cramer's rule:

$$
\begin{aligned}
\Phi_{2 c}^{J} & =\frac{\left|\begin{array}{cc}
\Phi_{2 c \max } & 1 \\
\Phi_{1 c \max } & \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}}
\end{array}\right|}{\left|\begin{array}{cc}
1 \\
\frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} & \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}}
\end{array}\right|}=\frac{\Phi_{2 c \max } \frac{\kappa_{2 c}^{2}-\lambda^{22}}{\kappa_{R c}^{2}}-\Phi_{1 c \max }}{\frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}}-\frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}}} \\
& =\frac{\Phi_{1 c \max } \kappa_{R c}^{2}-\Phi_{2 c \max }\left(\kappa_{2 c}^{2}-\lambda^{2}\right)}{\lambda^{2}+\mu^{2}}
\end{aligned}
$$

$$
\Phi_{2 c}^{I}=\frac{\left|\begin{array}{cc}
1 & \Phi_{2 c \max } \\
\frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} & \Phi_{1 c \max }
\end{array}\right|}{\left|\begin{array}{ccc}
1 \\
\frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} & \frac{\kappa_{2 c}^{2}}{\kappa_{R c}^{2}} & \lambda^{2} \\
\kappa_{R c}^{2}
\end{array}\right|}=\frac{\Phi_{1 c \max }-\Phi_{2 c \max } \frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}}}{\frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}}-\frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}}}
$$

$$
=\frac{\Phi_{2 c \max }\left(\kappa_{2 c}^{2}+\lambda^{2}\right)-\Phi_{1 c \max } \kappa_{R c}^{2}}{\lambda^{2}+\mu^{2}}
$$

### 13.4.4 Flux in the Reflector

Let us recall the flux equations in the reflector:

$$
\left\{\begin{array}{c}
\Delta \Phi_{1 r}(r)-\kappa_{1 r}^{2} \Phi_{1 r}(r)=0 \\
\Delta \Phi_{2 r}(r)-\kappa_{2 r}^{2} \Phi_{2 r}(r)=-\frac{\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(r)}{D_{2 r}}=-\kappa_{R r}^{2} \Phi_{1 r}(r)
\end{array}\right.
$$

The general solution to the fast flux equation is written as: $\Phi_{1 r}(r)=\Phi_{1 r}^{I} I_{0}\left(\kappa_{1 r} r\right)+\Phi_{1 r}^{K} K_{0}\left(\kappa_{1 r} r\right)$. It can be immediately seen that $\Phi_{1 r}^{I}=0$
since flux tends towards 0 at infinity. $\Phi_{1 r}^{K}$ may be expressed in terms of $\Phi_{1 c \max }$ and $\Phi_{2 c \text { max }}$ using the flux continuity at the interface $R$ :
$\Phi_{1 r}(R)=\Phi_{1 r}^{K} K_{0}\left(\kappa_{1 r} R\right)=\Phi_{1 r}(R)=\Phi_{2 c}^{J} \frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} J_{0}(\mu R)+\Phi_{2 c}^{I} \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}} I_{0}(\lambda R)$
Thus:

$$
\Phi_{1 r}^{K}=\Phi_{2 c}^{J} \frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} \frac{J_{0}(\mu R)}{K_{0}\left(\kappa_{1 r} R\right)}+\Phi_{2 c}^{I} \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}} \frac{I_{0}(\lambda R)}{K_{0}\left(\kappa_{1 r} R\right)}
$$

Clearly, coefficient $\Phi_{1 r}^{K}$ must be positive to ensure that the flux solution is positive in the reflector. The thermal flux solution is sought as $\Phi_{2 r}(r)=\Phi_{2 r}^{I} I_{0}\left(\kappa_{2 r} r\right)+\Phi_{2 r}^{K} K_{0}\left(\kappa_{2 r} r\right)+\Psi_{2 r}^{K} K_{0}\left(\kappa_{1 r} r\right)$. Since the thermal flux also tends towards 0 as $r$ tends to infinity, $\Phi_{2 r}^{I}=0$. The values of $\Phi_{2 r}^{K}$ and $\Psi_{2 r}^{K}$ are obtained by substituting the thermal flux expression in the differential equation:

$$
\begin{aligned}
\Delta \Phi_{2 r}(r)-\kappa_{2 r}^{2} \Phi_{2 r}(r) & =\frac{1}{r} \frac{d}{d r}\left(r \frac{d \Phi_{2 r}(r)}{d r}\right)-\kappa_{2 r}^{2} \Phi_{2 r}(r) \\
& =-\kappa_{R r}^{2} \Phi_{1 r}(r)=-\kappa_{R r}^{2} \Phi_{1 r}^{K} K_{0}\left(\kappa_{1 r} r\right)
\end{aligned}
$$

Leading to: $\Delta K_{0}\left(\kappa_{2 r} r\right)=\kappa_{2 r}^{2} K_{0}\left(\kappa_{2 r} r\right)$ and $\Delta K_{0}\left(\kappa_{1 r} r\right)=\kappa_{1 r}^{2} K_{0}\left(\kappa_{1 r} r\right)$
Therefore:

$$
\begin{aligned}
\Delta \Phi_{2 r}(r)-\kappa_{2 r}^{2} \Phi_{2 r}(r)= & \underbrace{\Phi_{2 r}^{K} \Delta K_{0}\left(\kappa_{2 r} r\right)-\kappa_{2 r}^{2} \Phi_{2 r}^{K} K_{0}\left(\kappa_{2 r} r\right)}_{0}+\Psi_{2 r}^{K} \Delta K_{0}\left(\kappa_{2 r} r\right) \\
& -\kappa_{2 r}^{2} \Psi_{2 r}^{K} K_{0}\left(\kappa_{1 r} r\right)=-\kappa_{R r}^{2} \Phi_{1 r}^{K} K_{0}\left(\kappa_{1 r} r\right)
\end{aligned}
$$

thereby: $\quad \Psi_{2 r}^{K}=\Phi_{1 r}^{K} \frac{\kappa_{R r}^{2}}{\kappa_{2 r}^{2}-\kappa_{1 r}^{2}}$
The continuity for the thermal flux at $R$ enables determination of $\Phi_{2 r}^{K}$ :

$$
\begin{gathered}
\Phi_{2 r}(R)=\Phi_{2 r}^{K} K_{0}\left(\kappa_{2 r} R\right)+\Psi_{2 r}^{K} K_{0}\left(\kappa_{1 r} R\right)=\Phi_{2 c}(R)=\Phi_{2 c}^{J} J_{0}(\mu R)+\Phi_{2 c}^{I} I_{0}(\lambda R) \\
\Phi_{2 r}^{K}=\frac{1}{K_{0}\left(\kappa_{2 r} R\right)}\left(\Phi_{2 c}^{J} J_{0}(\mu R)+\Phi_{2 c}^{I} I_{0}(\lambda R)-\Psi_{2 r}^{K} K_{0}\left(\kappa_{1 r} R\right)\right)
\end{gathered}
$$

Finally giving:
Flux in the reflector:

$$
\left\{\begin{array}{c}
\Phi_{1 r}(r)=\left(\Phi_{2 c}^{J} \frac{\kappa_{2 c}^{2}+\mu^{2}}{\kappa_{R c}^{2}} \frac{J_{0}(\mu R)}{K_{0}\left(\kappa_{1 r} R\right)}+\Phi_{2 c}^{I} \frac{\kappa_{2 c}^{2}-\lambda^{2}}{\kappa_{R c}^{2}} \frac{I_{0}(\lambda R)}{K_{0}\left(\kappa_{1 r} R\right)}\right) K_{0}\left(\kappa_{1 r} r\right)  \tag{13.21}\\
\Phi_{2 r}(r)=\frac{1}{K_{0}\left(\kappa_{2 r} R\right)}\left(\Phi_{2 c}^{J} J_{0}(\mu R)+\Phi_{2 c}^{I} I_{0}(\lambda R)-\Psi_{2 r}^{K} K_{0}\left(\kappa_{1 r} R\right)\right) K_{0}\left(\kappa_{2 r} r\right)+\Phi_{1 r}^{K} \frac{\kappa_{R r}^{2}}{\kappa_{2 r}^{2}-\kappa_{1 r}^{2}} K_{0}\left(\kappa_{1 r} r\right)
\end{array}\right.
$$

Study of these two functions shows that if the fast flux is a decreasing function in $r$, the thermal flux on the other hand increases, given that the decrease in the fast flux drives the thermal flux (Lamarsh and Barrata 2001, p. 305). Mathematically, this is due to the fact that the functions $K_{0}\left(\kappa_{2 r} r\right)$ and $K_{0}\left(\kappa_{1 r} r\right)$ do not decrease at the same "rate". It should be noted that (Fig. 13.10):

$$
\kappa_{1 r}^{2}=\Sigma_{t_{1 r}} / D_{1 r}=1 / L_{1 r}^{2}<\kappa_{2 r}^{2}=\Sigma_{t_{2 r} r} / D_{2 r}=1 / L_{2 r}^{2}
$$

since $L_{1 r}^{2} \approx 4 L_{2 r}^{2}$.
Since $\Phi_{2}^{r}(r)=-\alpha^{2} K_{0}\left(\kappa_{2 r} r\right)+\beta^{2} K_{0}\left(\kappa_{1 r} r\right)$, decay of the negative term $-\alpha^{2}$ $K_{0}\left(\kappa_{2 r} r\right)$ leads to a rise in the thermal flux that is very characteristic of thermalneutron reactors. The criticality condition is expressed using the current continuity equations at the interface, as illustrated in the simpler cases. The idea is to cancel out the constant terms with the flux continuity equations and this calculation poses no theoretical difficulty. Because of the continuity of the fast current, a large value of the fast diffusion coefficient for the reflector induces a rapid decay of the fast flux close to the reflector. Due to the coupling with the thermal equations for the fuel, the thermal flux rises. This effect illustrates the fact that the reflector directs some of the fast neutrons back into the core after thermalizing them. The reflector consequently acts as a biological protection barrier as well as a structure that economizes on fissile material, thereby explaining its importance in reactor physics.

Fig. 13.10 Two-group flux in a cylinder with an infinite reflector


### 13.5 Slab Reactor with Finite Reflector and Without Up-Scattering

The slab reactor is representative of several realistic configurations such as the upper and lower reflectors, or even the radial reflector of large pseudo-cylindrical reactors. Assuming that the slab reactor of thickness $a$ is surrounded by a slab reflector of thickness $b$ on each side (Fig. 13.11), the two-group diffusion equations for the fuel zone are expressed as:
$\left\{\begin{array}{l}-D_{1 c} \frac{d^{2} \Phi_{1 c}(x)}{d x^{2}}+\Sigma_{1, c} \Phi_{1 c}(x)=\frac{\nu \Sigma_{f_{1 c}} \Phi_{1 c}(x)+\nu \Sigma_{f_{2 c}} \Phi_{2 c}(x)}{k_{e f f}} \text { in the fast group } \\ -D_{2 c} \frac{d^{2} \Phi_{2 c}(x)}{d x^{2}}+\Sigma_{a 2, c} \Phi_{2 c}(x)=\Sigma_{1 \rightarrow 2, c} \Phi_{1 c}(x) \quad \text { in the thermal group }\end{array}\right.$
In the reflector, there is no fission source:

$$
\left\{\begin{array}{c}
-D_{1 r} \frac{d^{2} \Phi_{1 r}(x)}{d x^{2}}+\Sigma_{1, r} \Phi_{1 r}(x)=0 \\
-D_{2 r} \frac{d^{2} \Phi_{2 r}(x)}{d x^{2}}+\Sigma_{a 2, r} \Phi_{2 r}(x)=\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(x)
\end{array} \quad \Sigma_{1, r} \equiv \Sigma_{a 1, r}+\Sigma_{1 \rightarrow 2, r}\right.
$$

and the usual flux and current continuity equations are written as:

$$
\left\{\begin{array}{lr}
\Phi_{c}\left(\frac{a}{2}\right)=\Phi_{r}\left(\frac{a}{2}\right) & \text { for both groups } \\
\Phi_{r}\left(\frac{a}{2}+b\right)=\Phi_{r}\left(-\left(\frac{a}{2}+b\right)\right)=0 & \\
D_{c}\left(\frac{d \Phi_{c}}{d x}\right)_{x=q / 2}=D_{r}\left(\frac{d \Phi_{r}}{d x}\right)_{x=\% / 2} & \text { also true for }-q / 2
\end{array}\right.
$$

Fig. 13.11 Slab reactor with two zones


The problem is simplified by observing that the fast fission rate is negligible compared to the thermal fission rate in thermal-neutron reactors, i.e.: $\nu \Sigma_{f_{1}}^{c} \Phi_{1 c} \ll \nu \Sigma_{f_{2}}^{c} \Phi_{2 c}$. This approximation is useful to uncouple the calculation of the fast flux in the fuel from that for the thermal flux. From the thermal equation, the following relation is deduced

$$
\Phi_{1 c}=-\frac{D_{2 c}}{\Sigma_{1 \rightarrow 2, c}} \frac{d^{2} \Phi_{2 c}}{d x^{2}}+\frac{\Sigma_{a 2, \mathrm{c}} \Phi_{2 c}}{\Sigma_{1 \rightarrow 2, c}}
$$

which is inserted in the fast equation to give:
$\frac{D_{1 c} D_{2 c}}{\Sigma_{1, c} \Sigma_{a 2, c}} \frac{d^{4} \Phi_{2 c}}{d x^{4}}-\left(\frac{D_{1 c}}{\Sigma_{1, c}}+\frac{D_{2 c}}{\Sigma_{a 2, c}}\right) \frac{d^{2} \Phi_{2 c}}{d x^{2}}-\left(\frac{\nu \Sigma_{f_{2 c}}}{k_{e f f} \Sigma_{a 2, c}} \frac{\Sigma_{1 \rightarrow 2, c}}{\Sigma_{1, c}}-1\right) \Phi_{2 c}=0$
Setting: $\quad \frac{d^{2} F(x)}{d x^{2}}+\mu^{2} F(x)=0 \quad$ with: $\quad F(x)=\frac{d^{2} \Phi_{2 c}}{d x^{2}}-\lambda^{2} \quad \Phi_{2 c}(x)$
We identify: $\quad \lambda^{2} \mu^{2}=\left(\frac{\nu \Sigma_{f_{2 c}}}{k_{e f f} \Sigma_{1, c}} \frac{\Sigma_{1 \rightarrow 2, c}}{\Sigma_{a 2, c}}-1\right)\left(\frac{\Sigma_{1, c}}{D_{1 c}} \frac{\Sigma_{a 2, c}}{D_{2 c}}\right)$
and: $\quad \lambda^{2}-\mu^{2}=\frac{\Sigma_{1, c}}{D_{1 c}}+\frac{\Sigma_{a 2, c}}{D_{2 c}}$
The solution in slab geometry is a combination of $\cos (\mu x), \sin (\mu x), \operatorname{ch}(\lambda, x)$, $\operatorname{sh}(\lambda, x)$. From symmetry considerations $\left(\Phi_{2 c}(-x)=\Phi_{2 c}(x)\right), \Phi_{2 c}(x)=A \cos (\mu x)$ $+B \operatorname{ch}(\lambda x)$ is chosen.

Thus:

$$
\Phi_{1 c}(x)=C \quad \cos (\mu x)+D \operatorname{ch}(\lambda x)
$$

In strictly identical fashion, given that:

$$
\frac{\Sigma_{1 \rightarrow 2, r}}{\Sigma_{a 2, r}-D_{2 r} \frac{\Sigma_{1, c}}{D_{1 r}}} \Phi_{1 r}(x)
$$

is the particular solution for the thermal flux equation in the reflector, the complete solution for the thermal flux is computed as the sum of the particular solution to the inhomogeneous equation and the general solution to the homogeneous equation. Using the usual notations:

$$
\left\{\begin{array}{l}
\Phi_{1 r}(x)=E \operatorname{sh}\left(\frac{\frac{a}{2}+b-x}{L_{1 r}}\right) \\
\Phi_{2 r}(x)=F \operatorname{sh}\left(\frac{\frac{a}{2}+b-x}{L_{2 r}}\right)+\frac{\Sigma_{1 \rightarrow 2, r}}{\Sigma_{a 2, r}-\frac{D_{2 r}}{L_{1 r}^{2}}} \Phi_{1 r}(x)
\end{array}\right.
$$

The remaining constant coefficients are obtained using a closure relation, for example, the power produced by the reactor, with the same logic as the previous calculations for simple geometries already discussed.

### 13.6 The Ackroyd "Magic Shell" Albedo Model

At the beginning of the $1950 \mathrm{~s},{ }^{5}$ Ackroyd ${ }^{6}$ proposed a simple approach to calculate the albedo for a fast neutron reactor (refer to (Controle de la criticalité 1961, p. 57), which contains comparisons to experimental measurements). The active core is modeled using one-group (fast) diffusion theory while the reflector is dealt with using two-group theory.

The core may be thought of as being separated from the reflector by a thin layer of "black-body" medium which absorbs all thermal neutrons and produces $\eta$ fast neutrons, half of which return to the core while the others travel towards the reflector (Fig. 13.12). This layer has been called a "magic shell" due to its astonishing properties. Besides, a further situation to consider is that in which the "magic shell" and the reflector are grouped together. The following albedos are defined:

$$
\beta=\frac{J_{0 C}^{-}}{J_{0 C}^{+}} \quad \beta^{*}=\frac{J_{0 \cup}^{-}}{J_{0 \cup}^{+}}
$$

The first albedo is for a situation involving three zones, while the second is for the case in which the reflector and the magic shell are grouped together. Two probabilities are defined: $p_{1 \rightarrow 1}$ is the probability of a fast neutron entering the reflector and being reflected as a fast neutron, while $p_{2 \rightarrow 1}$ is the probability of a thermal neutron being reflected as a fast neutron by the reflector:

[^274]Fig. 13.12 "Magic shell" albedo model


$$
p_{1 \rightarrow 1}=\frac{J_{1 R}^{-}}{J_{1 R}^{+}} \quad p_{2 \rightarrow 1}=\frac{J_{2 R}^{-}}{J_{1 R}^{+}}
$$

It should be remarked that due to the properties of the black body, no thermal neutrons can escape the magic shell. The currents are related by:

$$
\left\{\begin{array}{l}
J_{1 R}^{+}=J_{0 \cup}^{+}+\frac{\eta}{2} J_{2 R}^{-} \\
J_{0 \cup}^{-}=J_{1 R}^{-}+\frac{\eta}{2} J_{2 R}^{-}
\end{array}\right.
$$

hence:

$$
\beta^{*}=\frac{J_{0 \cup}^{-}}{J_{0 \cup}^{+}}=\frac{J_{1 R}^{-}+\frac{\eta}{2} J_{2 R}^{-}}{J_{1 R}^{+}-\frac{\eta}{2} J_{2 R}^{-}}=\frac{p_{1 \rightarrow 1}+\frac{\eta}{2} p_{2 \rightarrow 1}}{1-\frac{\eta}{2} p_{2 \rightarrow 1}}
$$

The fast flux in the fuel is governed by the diffusion equation:

$$
\Delta \Phi_{0}+B_{m}^{2} \Phi_{0}=0 \quad \text { with } \quad B_{m}^{2}=\frac{\nu \Sigma_{f}-\Sigma_{a, 0}}{D_{0}}
$$

where the fast and thermal currents in the reflector satisfy:

$$
\begin{cases}\Delta \Phi_{1}-\kappa_{1}^{2} \Phi_{1}=0 & \text { with } \kappa_{1}^{2}=\frac{\Sigma_{a, 1}}{D_{1}} \\ \Delta \Phi_{2}-\kappa_{2}^{2} \Phi_{2}+\kappa_{r}^{2} \Phi_{1}=0 & \text { with } \quad \kappa_{2}^{2}=\frac{\Sigma_{a, 2}}{D_{2}} \quad \text { and } \quad \kappa_{r}^{2}=\frac{\Sigma_{1 \rightarrow 2}}{D_{2}}\end{cases}
$$

Table 13.2 "Magic shell" albedo for some reference geometries (Controle de la criticalité 1961, p. 59)

|  | $p_{1 \rightarrow 1}$ | $p_{2 \rightarrow 1}$ | $\beta$ |
| :--- | :--- | :--- | :--- |
| Slab $e=2 a$ | $\frac{1-2 D_{1} \kappa_{1}}{1+2 D_{1} \kappa_{1}}$ | $\frac{4 D_{1} \kappa_{1}}{\left(\kappa_{r}+\kappa_{1}\right)\left(1+2 D_{1} \kappa_{1}\right)\left(1+2 D_{2} \kappa_{r}\right)}$ | $\frac{1-2 D_{0} B_{m} \tan \left(B_{m} a\right)}{1+2 D_{0} B_{m} \tan \left(B_{m} a\right)}$ |
| Cylinder $R=a$ | $\frac{1-2 D_{1} \kappa_{1} \frac{K_{1}\left(B_{m} a\right)}{K_{0}\left(B_{m} a\right)}}{1+2 D_{1} \kappa_{1} \frac{K_{1}\left(B_{m} a\right)}{K_{0}\left(B_{m} a\right)}}$ | $\frac{4 D_{1} \kappa_{1}^{2}\left(\kappa_{2} \frac{K_{1}\left(B_{m} a\right)}{K_{0}\left(B_{m} a\right)}-\kappa_{1} \frac{K_{1}\left(B_{m} a\right)}{K_{0}\left(B_{m} a\right)}\right)}{\left(\kappa_{r}^{2}-\kappa_{1}^{2}\right)\left(1+2 D_{1} \kappa_{1} \frac{K_{1}\left(B_{m} a\right)}{K_{0}\left(B_{m} a\right)}\right)\left(1+2 D_{2} \kappa_{2} \frac{K_{1}\left(B_{m} a\right)}{K_{0}\left(B_{m} a\right)}\right)}$ | $\frac{1-2 D_{0} B_{m} \frac{J_{1}\left(B_{m} a\right)}{J_{0}\left(B_{m} a\right)}}{1+2 D_{0} B_{m} \frac{J_{1}\left(B_{m} a\right)}{J_{0}\left(B_{m} a\right)}}$ |
| Sphere $R=a$ | $\frac{1-2 D_{1} \frac{\kappa_{1} a+1}{a}}{1+2 D_{1} \frac{\kappa_{1} a+1}{a}}$ | $\frac{4 D_{1} \kappa_{1}}{\left(\kappa_{r}+\kappa_{1}\right)\left(1+2 D_{1} \frac{\kappa_{1} a+1}{a}\right)\left(1+2 D_{2} \frac{\kappa_{2} a+1}{a}\right)}$ | $\frac{a+2 D_{0}\left(B_{m} a \operatorname{cotan}\left(B_{m} a\right)-1\right)}{a-2 D_{0}\left(B_{m} a \operatorname{cotan}\left(B_{m} a\right)-1\right)}$ |

The criticality condition using the albedo method is evaluated by equating the fast neutron currents in the core and those from the homogenized medium consisting of the reflector and the magic shell, which is equivalent to equating the albedos:

$$
\beta=\frac{J_{0 C}^{-}}{J_{0 C}^{+}}=\frac{J_{0 \cup}^{-}}{J_{0 \cup}^{+}}=\beta^{*}
$$

Calculation for different geometries (a slab of thickness $2 a$, a cylinder of radius $a$, and a sphere of radius $a$ ) gives the formulae provided in Table 13.2:

This method, which is very simple, nevertheless underestimates the distance travelled by fast neutrons in the reflector and tends to underestimate the critical mass.

### 13.7 The Lefebvre-Lebigot Reflector Model

The Lefebvre-Lebigot model is the historical in-house reflector model used at EDF for two energy group diffusion calculations (thermal cut-off at 0.625 eV ). The choice of thermal cut-off at 0.625 eV is itself a historical choice that is widely used, even at the international level, and corresponds to the cadmium cut-off point. This value is often associated with the fact that up-scattering from the thermal energy group towards the fast group is not modeled. The equations are thus simplified since the fast flux equation becomes independent of the thermal equation. Nonetheless, it should be noted that physically, up-scattering occurs, even above 0.625 eV , since neutrons may up-scatter to energies of 2.72 eV . The Lefebvre-Lebigot model is based on this cut-off approach: it is a slab geometry model with a cut-off at 0.625 eV and without up-scattering. Nevertheless, this relatively simple model has been thoroughly tested for the calculation of loading patterns in nominal working conditions.

### 13.7.1 "Equivalent" Reflectors Theory

The Lefebvre-Lebigot ${ }^{7}$ model, conceived in the 1970s, is based on slab geometry. The goal is to conserve the ratio of neutron quantities for an "equivalent" reflector calculated in diffusion theory with respect to a full transport reference calculation: thermal flux to fast flux, thermal current to fast current, and fast current to fast flux at the core/reflector interface. The neutron quantities may have non-physical values, i.e. they do not have the expected values for a reflector with a given isotopic composition. Thus, this equivalent reflector is a mathematical reflector. The two-group diffusion equations without up-scattering are written as:

$$
\left\{\begin{array}{c}
-D_{1 r} \frac{d^{2} \Phi_{1 r}(x)}{d x^{2}}+\Sigma_{1, r} \Phi_{1 r}(x)=0 \\
-D_{2 r} \frac{d^{2} \Phi_{2 r}(x)}{d x^{2}}+\Sigma_{a 2, r} \Phi_{2 r}(x)=\Sigma_{1 \rightarrow 2, r} \Phi_{1 r}(x)
\end{array}\right.
$$

with

$$
\Sigma_{1, r} \equiv \Sigma_{a_{1} r}+\Sigma_{1 \rightarrow 2, r}
$$

which are expressed in the canonical form:

$$
\left\{\begin{array} { c } 
{ \frac { d ^ { 2 } \Phi _ { 1 r } } { d x ^ { 2 } } - \frac { 1 } { L _ { 1 r } ^ { 2 } } \Phi _ { 1 r } ( x ) = 0 } \\
{ \frac { d ^ { 2 } \Phi _ { 2 r } } { d x ^ { 2 } } - \frac { 1 } { L _ { 2 r } ^ { 2 } } \Phi _ { 2 r } ( x ) = - \frac { 1 } { L _ { R r } ^ { 2 } } \Phi _ { 1 r } ( x ) }
\end{array} \text { with } \left\{\begin{array}{l}
L_{1 r}^{2}=\frac{D_{1 r}}{\sum_{1, r}}=\frac{1}{\kappa_{1 r}^{2}} \\
L_{2 r}^{2}=\frac{D_{2 r}}{\sum_{a 2, r}}=\frac{1}{\kappa_{2 r}^{2}}
\end{array} \text { and } L_{R r}^{2}=\frac{D_{2 r}}{\sum_{1 \rightarrow 2, r}}=\frac{1}{\kappa_{R r}^{2}}\right.\right.
$$

The solution for the fast flux equation in the reflector is trivial for the flux that cancels to zero ad infinitum (using the reference of the $x$-axis at the core/reflector interface):

$$
\Phi_{1 r}(x)=\Phi_{1 r}(0) e^{-\kappa_{1 r} x}
$$

The thermal flux is easily obtained under the form $\Phi_{2 r}(x)=\Phi_{2 r}^{-} e^{-\kappa_{1 r} x}+\Psi_{2 r}^{-} e^{-\kappa_{2 r} x}$. Inserting this flux solution in the differential equation for the thermal flux gives:

[^275]$$
\frac{d^{2}\left[\Phi_{2 r}^{-} e^{-\kappa_{1 r} x}+\Psi_{2 r}^{-} e^{-\kappa_{2 r} x}\right]}{d x^{2}}-\kappa_{2 r}^{2}\left[\Phi_{2 r}^{-} e^{-\kappa_{1 r} x}+\Psi_{2 r}^{-} e^{-\kappa_{2 r} x}\right]=-\kappa_{R r}^{2} \Phi_{1 r}(0) e^{-\kappa_{1 r} x}
$$
thus:
$$
\Phi_{2 r}^{-}=\frac{\kappa_{R r}^{2}}{\left[\kappa_{2 r}^{2}-\kappa_{1 r}^{2}\right]} \Phi_{1 r}(0)
$$

The coefficient $\Psi_{2 r}^{-}$is computed using the boundary condition: $\Phi_{2 r}(0)=\Phi_{2 r}^{-}+\Psi_{2 r}^{-}$. Finally the fast and thermal fluxes in the reflector are obtained as:

Fluxes in the reflector:

$$
\left\{\begin{array}{c}
\Phi_{1 r}(x)=\Phi_{1 r}(0) e^{-\kappa_{1 r} x}  \tag{13.22}\\
\Phi_{2 r}(x)=\frac{\kappa_{R r}^{2}}{\left[\kappa_{2 r}^{2}-\kappa_{1 r}^{2}\right]} \Phi_{1 r}(0) e^{-\kappa_{1 r} x}+\left[\Phi_{2 r}(0)-\frac{\kappa_{R r}^{2}}{\left[\kappa_{2 r}^{2}-\kappa_{1 r}^{2}\right]} \Phi_{1 r}(0)\right] e^{-\kappa_{2 r} x}
\end{array}\right.
$$

Currents in diffusion theory are given by:

$$
\left\{\begin{array}{c}
J_{1 r}(0)=-D_{1 r} \operatorname{grad}\left(\Phi_{1 r}(x)\right)_{0}=\frac{D_{1 r}}{L_{1 r}} \Phi_{1 r}(0) \\
J_{2 r}(0)=-D_{2 r} \operatorname{grad}\left(\Phi_{2 r}(x)\right)_{0}=\frac{D_{2 r}}{L_{1 r}} \frac{\kappa_{R r}^{2}}{\left[\kappa_{2 r}^{2}-\kappa_{1 r}^{2}\right]} \Phi_{1 r}(0)+\frac{D_{2 r}}{L_{2 r}}\left[\Phi_{2 r}(0)-\frac{\kappa_{R r}^{2}}{\left[\kappa_{2 r}^{2}-\kappa_{1 r}^{2}\right]} \Phi_{1 r}(0)\right]
\end{array}\right.
$$

which can be expressed in the simplified canonical form as:
Characteristic equations for the reflector:

$$
\left\{\begin{array}{c}
\frac{J_{1 r}(0)}{\Phi_{1 r}(0)}=\frac{D_{1 r}}{L_{1 r}}  \tag{13.23}\\
\frac{J_{2 r}(0)}{\Phi_{1 r}(0)}=-\frac{L_{1 r} L_{2 r} \Sigma_{1 \rightarrow 2, r}}{\left(L_{1 r}+L_{2 r}\right)}+\frac{D_{2 r}}{L_{2 r}} \frac{\Phi_{2 r}(0)}{\Phi_{1 r}(0)}
\end{array}\right.
$$

The spectrum index at the interface, defined as the ratio of the thermal flux to the fast flux, is introduced as a correlating quantity of the ratio of the thermal current to the fast current. Hence, the characteristic functions of the reflector are plotted as two straight lines that are functions of the spectrum index (Fig. 13.13).

The two-group fuel diffusion equations without up-scattering are written as:

$$
\left\{\begin{array}{c}
-D_{1 c} \frac{d^{2} \Phi_{1 c}}{d x^{2}}+\Sigma_{1, c} \Phi_{1 c}=\frac{\nu \Sigma_{f_{1}}^{c} \Phi_{1 c}+\nu \Sigma_{f_{2}}^{c} \Phi_{2 c}}{k_{e f f}} \\
-D_{2 c} \frac{d^{2} \Phi_{2 c}}{d x^{2}}+\Sigma_{a 2, c} \Phi_{2 c}=\Sigma_{1 \rightarrow 2, c} \Phi_{1 c}
\end{array} \text { with } \Sigma_{1, c}=\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}\right.
$$



Fig. 13.13 Two-group characteristic functions without up-scattering for a neutron reflector

In the second equation, $\Phi_{1 c}$ is expressed in terms of $\Phi_{2 c}$ and inserted in the first equation to obtain an equation with the fast flux derivative:

$$
\begin{aligned}
& {\left[\frac{D_{2 c} D_{1 c} k_{e f f}}{\nu \Sigma_{f_{2}}^{c}}\right] \frac{d^{4} \Phi_{1 c}}{d x^{4}}-\left[\frac{\Sigma_{a 2, c} D_{1 c} k_{e f f}}{\nu \Sigma_{f_{2}}^{c}}+D_{2 c} \frac{k_{e f f} \Sigma_{1, c}-\nu \Sigma_{f_{1}}^{c}}{\nu \Sigma_{f_{2}}^{c}}\right] \frac{d^{2} \Phi_{1 c}}{d x^{2}}} \\
& -\left[\Sigma_{1 \rightarrow 2, c}-\Sigma_{a 2, c} \frac{k_{e f f} \Sigma_{1, c}-\nu \Sigma_{f_{1}}^{c}}{\nu \Sigma_{f_{2}}^{c}}\right] \Phi_{1 c}=0
\end{aligned}
$$

As discussed previously, this differential equation can be solved in two steps: first, we seek a function $F$ such that:

$$
F(x)=\frac{d^{2} \Phi_{1 c}(x)}{d x^{2}}+\beta^{2} \Phi_{1 c}(x) \text { that, next, satisfies : } \frac{d^{2} F(x)}{d x^{2}}-\chi^{2} F(x)=0 .
$$

The parameters $\beta$ and $\chi$ are evaluated by the identification by comparison of the two fourth-order differential equations:

$$
\begin{gathered}
\frac{d^{2}\left[\frac{d^{2} \Phi_{1 c}(x)}{d x^{2}}+\beta^{2} \Phi_{1 c}(x)\right]}{d x^{2}}-\chi^{2}\left[\frac{d^{2} \Phi_{1 c}(x)}{d x^{2}}+\beta^{2} \Phi_{1 c}(x)\right] \\
\quad=\frac{d^{4} \Phi_{1 c}(x)}{d x^{4}}+\left[\beta^{2}-\chi^{2}\right] \frac{d^{2} \Phi_{1 c}(x)}{d x^{2}}-\beta^{2} \chi^{2} \Phi_{1 c}(x)
\end{gathered}
$$

Ultimately, the general solution for the fast fuel flux is expressed in the form:

$$
\Phi_{1 c}(x)=A \operatorname{ch}(\chi x)+B \operatorname{sh}(\chi x)+C \cos (\beta x)+D \sin (\beta x)
$$

using the center of the reactor as the origin coordinates. This expression may be readily simplified by noting that the flux is even in the fuel, and the sine and hyperbolic sine terms are cancelled. In addition, the coefficients $A$ and $C$ are related
using the boundary condition at the center of the reactor by normalizing the flux as $\Phi_{1 c}^{\max }=\Phi_{1 c}(0)$. Hence:

$$
\Phi_{1 c}(x)=\left(\Phi_{1 c}^{\max }-A\right) \cos (\beta x)+A \operatorname{ch}(\chi x)
$$

The thermal flux can also be written as: $\Phi_{2 c}(x)=E \cos (\beta x)+F \operatorname{ch}(\chi x)$. The constants $E$ and $F$ are expressed in terms of $A$ and of the fuel material properties by inserting the flux solutions in the thermal equation, i.e.:

$$
\begin{aligned}
& \left.-D_{2 c} \frac{d^{2}\left[\begin{array}{lll}
E & \cos (\beta x)+F & \operatorname{ch}(\chi x)]
\end{array}+\Sigma_{a 2, c}\left[\begin{array}{ll}
E & \cos (\beta x)+F \\
d x^{2} & c h(\chi x)
\end{array}\right]\right.}{\quad=\Sigma_{1 \rightarrow 2, c}\left[\left(\Phi_{1 c}^{\max }-A\right)\right.} \cos (\beta x)+A \operatorname{ch}(\chi x)\right]
\end{aligned}
$$

thus, the thermal flux is:

$$
\Phi_{2 c}(x)=\frac{\Sigma_{1 \rightarrow 2, c}}{D_{2 c} \beta^{2}+\Sigma_{a 2, c}}\left(\Phi_{1 c}^{\max }-A\right) \quad \cos (\beta x)+\frac{\Sigma_{1 \rightarrow 2, c}}{\Sigma_{a 2, c}-D_{2 c \chi^{2}}} A \quad \operatorname{ch}(\chi x)
$$

Employing the historical notations of Lefebvre and Lebigot, the equations are:

$$
\left\{\begin{array}{ll}
\Phi_{1 c}(x)=\left(\Phi_{1 c}^{\max }-A\right) \cos (\beta x)+A \operatorname{ch}(\chi x) & \text { with } \quad s=\frac{\Sigma_{1 \rightarrow 2, c}}{D_{2 c} \beta^{2}+\Sigma_{a 2, c}} \\
\Phi_{2 c}(x)=s\left(\Phi_{1 c}^{\max }-A\right) \cos (\beta x)+t A & \operatorname{ch}(\chi x)
\end{array} \quad \text { with } \quad t=\frac{\Sigma_{1 \rightarrow 2, c}}{-D_{2 c \chi^{2}+\Sigma_{a 2, c}}}\right.
$$

Using the forms of the fast and thermal flux introduced in the diffusion equations for the fuel and the reflector, the constants $A, \beta$ and $\chi$ are related as follows:

Eliminating $s$ from the equation in $\beta$ results in:

$$
D_{1 c} \beta^{2}+\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}-\frac{\nu \Sigma_{f_{1}}^{c}}{k_{e f f}}=\frac{\nu \Sigma_{f_{2}}^{c}}{k_{e f f}}\left[\frac{\Sigma_{1 \rightarrow 2, c}}{D_{2 c}} \beta^{2}+\Sigma_{a 2, c}\right]
$$

which Lefebvre and Lebigot express as a critical ${ }^{8}$ determinant corresponding to a quadratic equation in $\mu$ for which $\beta^{2}$ is a solution:

$$
\left|\begin{array}{ccc}
D_{1 c} \mu+\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}-\frac{\nu \Sigma_{f_{1}}^{c}}{k_{e f f}} & -\frac{\nu \Sigma_{f_{2}}^{c}}{k_{e f f}} \\
-\Sigma_{1 \rightarrow 2, c} & D_{2 c} & \mu+\Sigma_{a 2, c}
\end{array}\right|=0
$$

Similarly, eliminating $t$ from the equation in $\chi$ gives:

$$
-D_{1 c} \chi^{2}+\Sigma_{1, c}=\frac{\nu \Sigma_{f_{1}}^{c}+\nu \Sigma_{f_{2}}^{c}\left(\frac{\Sigma_{1-2, c}}{-D_{2 c} \chi^{2}+\Sigma_{a 2, c}}\right)}{k_{e f f}}
$$

Parameters $t$ and $-\chi^{2}$ have the same function as $s$ and $\beta^{2}$ in the previous equations since this equation may also be written as:

$$
-D_{1 c} \chi^{2}+\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}-\frac{\nu \Sigma_{f_{1}}^{c}}{k_{e f f}}=\frac{\nu \Sigma_{f_{2}}^{c}}{k_{e f f}}\left(\frac{\Sigma_{1 \rightarrow 2, c}}{-D_{2 c} \chi^{2}+\Sigma_{a 2, c}}\right)
$$

The coefficients $\beta^{2}$ and $-\chi^{2}$ are thus solutions to the critical determinant:

$$
\begin{gathered}
D_{1 c} D_{2 c} \mu^{2}+\left[\left(\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}-\frac{\nu \Sigma_{f_{1}}^{c}}{k_{e f f}}\right) D_{2 c}+D_{1 c} \Sigma_{a 2, c}\right] \mu \\
-\frac{\nu \Sigma_{f_{2}}^{c}}{k_{e f f}} \Sigma_{1 \rightarrow 2, c}+\left(\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}-\frac{\nu \Sigma_{f_{1}}^{c}}{k_{e f f}}\right) \Sigma_{a 2, c}=0
\end{gathered}
$$

This equation can be expressed in the canonical form using the equation that relates $\kappa_{\infty}$ to the fuel properties. In an infinite medium without leakage, the following equation is obtained:

$$
-\frac{\nu \Sigma_{f_{2}}^{c}}{k_{\infty}} \Sigma_{1 \rightarrow 2, c}+\left(\Sigma_{a 1, c}+\Sigma_{1 \rightarrow 2, c}-\frac{\nu \Sigma_{f_{1}}^{c}}{k_{\infty}}\right) \Sigma_{a 2, c}=0
$$

[^276]Therefore, the critical determinant can be written in the condensed form:

$$
\mu^{2}+\left(\frac{1}{L_{1 c}^{2}}+\frac{1}{L_{2 c}^{2}}-\frac{\nu \Sigma_{f_{1}}^{c}}{D_{1 c} k_{e f f}}\right) \mu+\left(\frac{\nu \Sigma_{f_{2}}^{c} \Sigma_{1 \rightarrow 2, c}+\nu \Sigma_{f_{1}}^{c} \Sigma_{a 2, c}}{D_{1 c} D_{2 c}}\right)\left(\frac{1}{k_{\infty}}-\frac{1}{k_{e f f}}\right)=0
$$

with: $\quad k_{\infty}=\frac{\nu \Sigma_{f_{1}}^{c} \Phi_{1 c}+\nu \Sigma_{f_{2}}^{c} \Phi_{2 c}}{\Sigma_{1, c} \Phi_{1 c}}=\frac{\nu \Sigma_{f_{1}}^{c}}{\Sigma_{1, c}}+\frac{\nu \Sigma_{f_{2}}^{c} \Sigma_{1 \rightarrow 2, c}}{\Sigma_{1, c} \Sigma_{a 2, c}}$
The sum and product of the two roots of this equation are then equal to:

$$
\left\{\begin{array}{c}
\beta^{2}-\chi^{2}=-\left(\frac{1}{L_{1 c}^{2}}+\frac{1}{L_{2 c}^{2}}-\frac{\nu \Sigma_{f_{1}}^{c}}{D_{1 c} k_{e f f}}\right) \\
-\beta^{2} \chi^{2}=\left(\frac{\nu \Sigma_{f_{2}}^{c} \Sigma_{1 \rightarrow 2, c}+\nu \Sigma_{f_{1}}^{c} \Sigma_{a 2, c}}{D_{1 c} D_{2 c}}\right)\left(\frac{1}{k_{\infty}}-\frac{1}{k_{e f f}}\right)
\end{array}\right.
$$

In practice, for industrial reactors, $\beta^{2} \ll \chi^{2}$, thus:

$$
\left\{\begin{array}{c}
\chi^{2} \approx \frac{1}{L_{1 c}^{2}}+\frac{1}{L_{2 c}^{2}}-\frac{\nu \Sigma_{f_{1}}^{c}}{D_{1 c} k_{e f f}} \\
\beta^{2}=\frac{\left(\nu \Sigma_{f_{2}}^{c} \Sigma_{1 \rightarrow 2, c}+\nu \Sigma_{f_{1}}^{c} \Sigma_{a 2, c}\right) L_{1 c}^{2} L_{2 c}^{2}}{D_{2 c}\left(k_{\infty} k_{e f f} D_{1 c} L_{2 c}^{2}+k_{\infty} k_{e f f} D_{1 c} L_{1 c}^{2}-\nu \Sigma_{f_{1}}^{c} k_{\infty} L_{1 c}^{2} L_{2 c}^{2}\right)}\left(k_{\infty}-k_{e f f}\right)>0
\end{array}\right.
$$

which can be inserted in the expressions of parameters $s$ and $t$.

### 13.7.2 Calculation of Core Characteristics

As for the reflector, the characteristic functions of the fuel core may be represented by the variation of the fast current to fast flux ratio and that of the thermal current to fast flux depending on the spectrum index. The boundary conditions for the flux and currents at the core/reflector interface (located at a distance $H$ from the center of the slab reactor) are written as:

$$
\left\{\begin{array}{l}
\Phi_{1 c}(H)=\left(\Phi_{1 c}^{\max }-A\right) \cos (\beta H)+A c h(\chi H) \\
\Phi_{2 c}(H)=s\left(\Phi_{1 c}^{\max }-A\right) \cos (\beta H)+t A \quad c h(\chi H) \\
J_{1 c}(x)=D_{1 c}\left(\left(\Phi_{1 c}^{\max }-A\right) \beta \sin (\beta H)-A \chi \operatorname{sh}(\chi H)\right) \\
J_{2 c}(x)=D_{2 c}\left(s\left(\Phi_{1 c}^{\max }-A\right) \beta \sin (\beta H)-t A \chi \quad \operatorname{sh}(\chi H)\right)
\end{array}\right.
$$

The following equations are deduced from the flux equations:
$\left(\Phi_{1 c}^{\max }-A\right) \cos (\beta H)=\frac{t \Phi_{1 c}(H)-\Phi_{2 c}(H)}{t-s} \quad$ and $A \operatorname{ch}(\chi H)=\frac{\Phi_{2 c}(H)-s \Phi_{1 c}(H)}{t-s}$
From the current equations, $\cos (\beta H)$ is introduced using $\sin (\beta H)=\operatorname{tg}(\beta H) \cos$ $(\beta H)$, and $\operatorname{ch}(\chi H)$ given that $\chi H \gg 1, \operatorname{ch}(\chi H) \approx \operatorname{sh}(\chi H)$ hence:

Thus, the fuel characteristics are evaluated as:
Fuel characteristics:

$$
\begin{cases}\frac{J_{1 c}(H)}{\Phi_{1 c}(H)} \approx \frac{D_{1 c}}{t-s}(t \beta \tan (\beta H)+s \chi) & -\frac{D_{1 c}}{t-s}(\beta \tan (\beta H)+\chi) \frac{\Phi_{2 c}(H)}{\Phi_{1 c}(H)}  \tag{13.24}\\ \frac{J_{2 c}(H)}{\Phi_{1 c}(H)}=\frac{D_{2 c}}{t-s} s t(\beta \tan (\beta H)+\chi) & -\frac{D_{2 c}}{t-s}(s \beta \tan (\beta H)+t \chi) \frac{\Phi_{2 c}(H)}{\Phi_{1 c}(H)}\end{cases}
$$

The characteristics are in fact decreasing lines in terms of the spectrum index at the interface (Fig. 13.14). The fast characteristic is decreasing and its slope increases as $\beta$ increases. The thermal characteristic is also decreasing but the slope remains globally constant as $\beta$ increases.

Lefebvre and Lebigot point out that the term $\beta \tan (\beta H)$ depends strongly on $k_{\text {eff }}$, but the latter can be eliminated by noting that:

$$
\left.\begin{array}{rl}
s \frac{D_{2 c}}{D_{1 c}} \frac{J_{1 c}(H)}{\Phi_{1 c}(H)}-\frac{J_{2 c}(H)}{\Phi_{1 c}(H)} & =\left[\begin{array}{ll}
-s D_{2 c} \chi & D_{2 c} \chi
\end{array} \frac{\Phi_{2 c}(H)}{\Phi_{1 c}(H)}\right.
\end{array}\right]
$$

However, $s$ is still dependent on $k_{\text {eff. }}$. At the core/reflector interface, flux and current continuity leads to:


Fig. 13.14 Effect of numerical coefficient $\beta$ (not to be confused with the albedo) on reflector characteristics

$$
\frac{J_{1 c}(H)}{\Phi_{1 c}(H)}=\frac{J_{1 r}(0)}{\Phi_{1 r}(0)}=\frac{D_{1 r}}{L_{1 r}}
$$

It may be seen that $J_{2 c}(H) / \Phi_{1 c}(H)$ is almost independent of $k_{\text {eff }}$ and flux shape $\beta^{2}$ (as long as $\beta^{2} \ll \chi^{2}$ ):

$$
\frac{J_{2 c}(H)}{\Phi_{1 c}(H)}=s\left[\frac{D_{2 c}}{D_{1 c}} \frac{D_{1 r}}{L_{1 r}}+D_{2 c} \chi\right]-D_{2 c} \chi\left[\frac{\Phi_{2 c}(H)}{\Phi_{1 c}(H)}\right]
$$

### 13.7.3 Core/Reflector Operating Point

The core/reflector operating point is defined as the intersection between the two characteristics such that $J_{c}(H) / \Phi_{1 c}(H)=J_{R}(H) / \Phi_{1 R}(H)$. Hence, even if the characteristic functions of the reflector are independent of the fuel driving zone, the operating point continues to depend on the core conditions (Fig. 13.15).

Finally, it may be seen that definition of the reflector characteristics hinges on defining three constants:

- first, the level of the horizontal line $\frac{J_{1 r}(0)}{\Phi_{1 r}(0)}$, i.e. the ratio $c=D_{1 r} / L_{1}$
- second, the equation of the line $\frac{J_{2 r}(0)}{\Phi_{1 r}(0)}=a \frac{\Phi_{2 r}(0)}{\Phi_{1 r}(0)}+b$, i.e. $b=-\frac{L_{1}, L_{2}, \Sigma_{1-2, r}}{\left(L_{1 r}+L_{2 r} r\right)}$ and $a=D_{2 r} / L_{2}$.

Given that in two-group diffusion theory without up-scattering, a reflector is completely defined by its properties $D_{1 r}, D_{2 r}, \Sigma_{a 1, r}, \Sigma_{a 2, r}, \Sigma_{1 \rightarrow 2, r}$, an infinite number of hypothetical reflectors is acceptable provided ratios $a, b$, and $c$ are conserved. Since there are three ratios to conserve and five unknowns or degrees of freedom, Lefebvre and Lebigot chose to set two degrees of freedom: $D_{1 r}$ and $D_{2 r}$,


Fig. 13.15 Graphical view of the core/reflector operating point
which are equated with the fuel diffusion coefficients, $D_{1 c}=1.3 \mathrm{~cm}$ and $D_{2 c}=0.4 \mathrm{~cm}$. The reflector thus obtained is a "mathematical" reflector that only conserves the core/reflector operating point at the interface but does not conserve the reaction rate inside the reflector itself. It is very important to understand that the neutron properties of the mathematical reflector do not correspond to those of a true (or "physical") reflector. The choice of equating the reflector diffusion coefficients with those of the fuel is purely arbitrary. Lefebvre and Lebigot justify their choice by arguing that they wished to avoid any "discontinuity" in the diffusion calculation for the reflector (in fact, the discontinuity on the flux gradients-which is physical in diffusion theory-is due to the discontinuity in the scattering properties of the materials). As a direct consequence, the fast and thermal flux inside the mathematical reflector are different from the true reflector, especially at the interface, where current continuity would be expressed as:

$$
\left\{\begin{array}{l}
J_{1 c}(H)=-D_{1 c} \operatorname{grad}(\left(\Phi_{1 c}(x)\right)_{H}=J_{1 R}(0)=-\underbrace{D_{1 r}}_{D_{1 c}} \operatorname{grad}\left(\left(\Phi_{1 r}(x)\right)_{0}\right. \\
J_{2 c}(H)=-D_{2 c} \operatorname{grad}(\left(\Phi_{2 c}(x)\right)_{H}=J_{1 R}(0)=-\underbrace{D_{2 r}}_{D_{2 c}} \operatorname{grad}\left(\left(\Phi_{2 r}(x)\right)_{0}\right.
\end{array}\right.
$$

hence the continuity of the flux gradients at the interface: $\operatorname{grad}\left(\left(\Phi_{1 c}(x)\right)_{H}=\operatorname{grad}\right.$ $\left(\left(\Phi_{1 r}(x)\right)_{0}\right.$ and $\operatorname{grad}\left(\left(\Phi_{2 c}(x)\right)_{H}=\operatorname{grad}\left(\left(\Phi_{2 r}(x)\right)_{0}\right.\right.$ for the mathematical reflector. Although the latter induces continuous flux gradients for the fast and thermal flux at the interface, nonetheless, the flux solutions consequently have no physical significance (Fig. 13.16). Nevertheless, the order of magnitude is conserved. Strictly speaking, the flux should not be calculated in the mathematical LefebvreLebigot reflector, but applied simply as an albedo condition that can be expressed under the matrix form of the Poincaré-Steklov operator (defined at the beginning of the chapter) as:


Fig. 13.16 Comparison of physical and mathematical reflectors in diffusion theory
Reflector transfer matrix:

$$
\binom{J_{1 r}(0)}{J_{2 r}(0)}=\underbrace{\left(\begin{array}{cc}
\frac{D_{1 r}}{L_{1}} & 0  \tag{13.25}\\
-\frac{L_{1}, L_{2 r} \Sigma_{1 \rightarrow 2, r}}{\left(L_{1, r}+L_{2 r}\right)} & \frac{D_{2 r}}{L_{2}}
\end{array}\right)}_{\Re}\binom{\Phi_{1 r}(0)}{\Phi_{2 r}(0)}
$$

The reflector transfer matrix $\mathfrak{R}$ is lower triangular since up-scattering is not considered. Taking up-scattering into account in the model gives a dense transfer matrix.

### 13.7.4 Effect of Thermal-Hydraulic Feedbacks

Lefebvre and Lebigot showed that the constants for the mathematical reflector are weakly impacted by the water density in the reflector. $D_{1 r}$ and $D_{2 r}$ are assumed to be constant and $\Sigma_{a 1, r}, \Sigma_{a 2, r}, \Sigma_{1 \rightarrow 2, r}$ have a variation of $1 \%$ when the water density varies by $5 \%$. In addition, they proved that the choice of the environment, $i . e$. the driver fuel zone, led to a $3 \%$ impact on $\Sigma_{a 1, r}, \Sigma_{a 2, r}, \Sigma_{1 \rightarrow 2, r}$ between the beginning and the end of life of the reactor. Only the effect of boron in the water of the reflector remains to be quantified and studies have shown that the sum $\Sigma_{a 1, r}+\Sigma_{1 \rightarrow 2, r}$ remains almost constant despite significant variation in boron concentration. However, $\Sigma_{a 2, r}$ is directly impacted by the boron concentration. Finally, feedback due to the latter is modeled as follows (Fig. 13.17):


Fig. 13.17 Comparison between the Lefebvre-Lebigot model (linear model) and the true values of the cross sections with boron concentration feedback (from a study by EDF research engineer Marie Fliscounakis). This comparison shows the robustness of the model [hashed lines $=$ linear model; unbroken lines $=$ true value with boron concentration feedback].

$$
\partial \Sigma_{a 1, r}=\sigma_{a 1, r} \partial N_{\text {boron }} \quad \partial \Sigma_{a 2, r}=\sigma_{a 2, r} \partial N_{\text {boron }} \quad \partial \Sigma_{1 \rightarrow 2, r}=-\partial \Sigma_{a 1, r}
$$

### 13.7.5 Calculation of Constants in the Mathematical Reflector

The characteristics of the mathematical reflector are calculated using three slab geometries for the core/reflector interface with a transport code. ${ }^{9}$ In the two initial calculations, the driver zone is modified to determine the characteristic lines at the interface (in configuration 1, close to a true core for which the spectrum index is close to 0.1 , and in configuration 2 for an over-moderated core for which the spectrum index is close to 0.2 ). The third calculation involves evaluating the dependence of the cross sections $\Sigma_{a 1, r}, \Sigma_{a 2, r}$ and eventually $\Sigma_{1 \rightarrow 2, r}$ (if the relation $\partial \Sigma_{1 \rightarrow 2, r}=-\partial \Sigma_{a 1, r}$ is not considered precise enough) on the boron concentration (Fig. 13.18).

Table 13.3 summarizes the neutron constants obtained using the LefebvreLebigot method for the reflectors of the three CPY reactors (with the boron macroscopic cross sections, the fraction of water Voliq and the water density). The fast diffusion coefficient of the reflector has been set to 1.78 cm instead of 1.3 cm on account of the significant experience of $E D F$ in improving radial power distribution.

[^277]| Fuel + water (dilution <br> $0.55)+500$ ppm boron | Baffle+water | Fuel <br> + water (dilution 0.7) | Baffle +water | Fuel <br> + water (dilution 0.7) |
| :---: | :---: | :---: | :---: | :--- |
| Baffle+water <br> +boron |  |  |  |  |
| configuration 1 | configuration 2 | configuration 3 |  |  |

Fig. 13.18 Configurations for the slab calculations to determine the operating point

Table 13.3 Neutron constants of the Lefebvre-Lebigot reflector for the CPY
\(\left.$$
\begin{array}{l|l|l|l|l|l|l|l|l|l}\hline & \begin{array}{l}D_{1 r} \\
{[\mathrm{~cm}]}\end{array} & \begin{array}{l}D_{2 r} \\
{[\mathrm{~cm}]}\end{array} & \begin{array}{l}\Sigma_{a 1 r} \\
{\left[\mathrm{~cm}^{-1}\right]}\end{array} & \begin{array}{l}\Sigma_{a 2 r} \\
{\left[\mathrm{~cm}^{-1}\right]}\end{array} & \begin{array}{l}\Sigma_{R r} \\
{\left[\mathrm{~cm}^{-1}\right]}\end{array} & \begin{array}{l}\sigma_{a 1}^{\text {Bore }} \\
{[\text { barn }]}\end{array}
$$ \& \begin{array}{l}\sigma_{a 2}^{Bore} <br>

{[barn]}\end{array} \& Voliq\end{array}\right\}\)| $\rho_{\mathrm{H}_{2} \mathrm{O}}^{\left[\mathrm{g} / \mathrm{cm}^{3}\right]}$ |
| :--- |

### 13.8 Albedo Matrix

In the earlier chapters, it was stated that the albedo is defined as the ratio of the outgoing current from the reflector to the incoming current towards the reflector $\beta=J^{-} / J^{+}$where $J^{-}$is the outgoing current and $J^{+}$is the incoming current. Given that in diffusion theory:

$$
J^{+}=\frac{1}{2}\left(\frac{\Phi}{2}+J\right) \quad J^{-}=\frac{1}{2}\left(\frac{\Phi}{2}-J\right)
$$

the following matrix can be written: $\quad\binom{J^{+}}{J^{-}}=\left(\begin{array}{cc}\frac{1}{4} & \frac{1}{2} \\ \frac{1}{4} & -\frac{1}{2}\end{array}\right)\binom{\Phi}{J}$
The current at the interface can also be written in the vector form $\left(J_{1 r}(0), J_{2 r}(0)\right)$, and is related to the flux by the transfer matrix $\mathfrak{R}$ as in Eq. (13.25). For two energy groups, the positive and negative currents may be expressed in terms of the flux as:

$$
\left\{\begin{array}{l}
\binom{J_{1}+}{J_{2}^{+}}=\frac{1}{2}\left[\frac{1}{2}\binom{\Phi_{1}}{\Phi_{2}}+\binom{J_{1}}{J_{2}}\right]=\frac{1}{2}\left[\left(\begin{array}{cc}
\frac{1}{2} & 0 \\
0 & \frac{1}{2}
\end{array}\right)+\left(\begin{array}{cc}
\frac{D_{1 r}}{L_{1 r}} & 0 \\
-\frac{L_{1 r} L_{2 r} \Sigma_{1 \rightarrow 2, r}}{\left(L_{1 r}+L_{2 r}\right)} & \frac{D_{2 r}}{L_{2 r}}
\end{array}\right)\right]\binom{\Phi_{1}}{\Phi_{2}} \\
\binom{J_{1}^{-}}{J_{2}^{-}}=\frac{1}{2}\left[\frac{1}{2}\binom{\Phi_{1}}{\Phi_{2}}-\binom{J_{1}}{J_{2}}\right]=\frac{1}{2}\left[\frac{1}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & 1
\end{array}\right)-\left(\begin{array}{cc}
\frac{D_{1 r}}{L_{1 r}} & 0 \\
-\frac{L_{1 r} L_{2 r} \Sigma_{1 \rightarrow 2, r}}{\left(L_{1 r}+L_{2 r}\right)} & \frac{D_{2 r}}{L_{2 r}}
\end{array}\right)\right]\binom{\Phi_{1}}{\Phi_{2}}
\end{array}\right.
$$

Substituting the flux by its value in terms of the positive current in the negative current equation leads to:

Thus, the albedo matrix ( $\beta_{\mathrm{ij}}$ ) may be introduced in the equation. The terms of the albedo matrix are calculated as follows:

Infinite albedo matrix:

$$
\binom{J_{1}^{-}}{J_{2}^{-}}=\underbrace{\left.\begin{array}{cc}
\frac{L_{1 r}-2 D_{1 r}}{L_{1 r}+2 D_{1 r}} & 0  \tag{13.26}\\
\frac{4\left(L_{1 r} L_{2 r}\right)^{2} \Sigma_{1 \rightarrow 2, r}}{\left(L_{1 r}+L_{2 r}\right)\left(L_{1 r}+2 D_{1 r}\right)\left(L_{2 r}+2 D_{2 r}\right)} & \frac{L_{2 r}-2 D_{2 r}}{L_{2 r}+2 D_{2 r}}
\end{array}\right)}_{\left(\beta_{i j}\right)^{\infty}}\binom{J_{1}^{+}}{J_{2}^{+}}
$$

This matrix is denoted by $\beta^{\infty}$, implying that it corresponds to a case in which the flux is zero at infinity. Assuming a zero flux at a finite distance (at the end of the reflector) entails a more complex albedo matrix and induces dependence on the size of the reflector. The albedo condition, which reproduces the reflector response accurately, can no longer be employed as such in exact transport theory or simplified transport theory with the $S P N$ with $N>1$. In the $S P 1$ method, equivalence with diffusion theory can be obtained $D=1 / 3 \Sigma_{\text {transport }}$ such that the albedo method can be used. Several models, very often $1 D$ models, have been set up, albeit with differing degrees of efficiency, to conserve the albedo matrix so that the constants are not impacted by the environment. ${ }^{10,11}$

### 13.9 Allowing for Up-Scattering

In the reflector, there is no fission source, yet with the up-scattering in energy hypothesis, there exists a source of fast neutrons through scattering from the thermal group to the fast group:

[^278]\[

\left\{$$
\begin{array} { l } 
{ - D _ { 1 r } \frac { d ^ { 2 } \Phi _ { 1 r } } { d x ^ { 2 } } + \Sigma _ { 1 , r } \Phi _ { 1 r } ( x ) = \Sigma _ { 2 \rightarrow 1 , r } \Phi _ { 2 r } ( x ) } \\
{ - D _ { 2 r } \frac { d ^ { 2 } \Phi _ { 2 r } } { d x ^ { 2 } } + \Sigma _ { 2 , r } \Phi _ { 2 r } ( x ) = \Sigma _ { 1 \rightarrow 2 , r } \Phi _ { 1 r } ( x ) }
\end{array}
$$ with \left\{$$
\begin{array}{l}
\Sigma_{1, r}=\Sigma_{a 1, r}+\Sigma_{1 \rightarrow 2, r} \\
\Sigma_{2, r}=\Sigma_{a 2, r}+\Sigma_{2 \rightarrow 1, r}
\end{array}
$$\right.\right.
\]

which, in the canonical form, gives:

$$
\begin{gathered}
\left\{\begin{array}{l}
\frac{d^{2} \Phi_{1 r}}{d x^{2}}-\frac{1}{L_{1 r}^{2}} \Phi_{1 r}(x)=-\frac{1}{L_{U r}^{2}} \Phi_{2 r}(x) \\
\frac{d^{2} \Phi_{2 r}}{d x^{2}}-\frac{1}{L_{2 r}^{2}} \Phi_{2 r}(x)=-\frac{1}{L_{R r}^{2}} \Phi_{1 r}(x)
\end{array}\right. \\
\text { with }\left\{\begin{array} { l } 
{ L _ { 1 r } ^ { 2 } = \frac { D _ { 1 r } } { \Sigma _ { 1 , r } } } \\
{ L _ { 2 r } ^ { 2 } = \frac { D _ { 2 r } } { \Sigma _ { 2 , r } } }
\end{array} \text { and } \left\{\begin{array}{l}
L_{U r}^{2}=\frac{D_{1 r}}{\Sigma_{2 \rightarrow 1, r}} \\
L_{R r}^{2}=\frac{D_{2 r}}{\Sigma_{1 \rightarrow 2, r}}
\end{array}\right.\right.
\end{gathered}
$$

From calculations analogous to the previous section, it can be shown that the fast flux satisfies the equation:

$$
\frac{d^{4} \Phi_{1 r}}{d x^{4}}-\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right] \frac{d^{2} \Phi_{1 r}}{d x^{2}}+\left[\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}\right] \Phi_{1 r}(x)=0
$$

The term $1 / L_{U r 2}$ might be expected be negligible if the cut-off between the two groups is at low energy values (the Lefebvre-Lebigot model assumes that there is no up-scattering). However, the term $1 / L_{R r 2}$, which represents the thermal neutron source term deriving from fast neutrons, is large. Finally, the term $\left[1 / L_{2 r}^{2} L_{1 r}^{2}-1 / L_{U r}^{2} L_{R r}^{2}\right]$ may be expected to be positive. This particular point will be illustrated later with numerical examples. Solving the equation thus obtained leads to a solution $F(x)$ such that:

$$
\begin{aligned}
F(x) & =\frac{d^{2} \Phi_{1 r}(x)}{d x^{2}}-\lambda^{2} \Phi_{1 r}(x) \quad \text { which furthermore satisfies }: \frac{d^{2} F(x)}{d x^{2}}-\mu^{2} F(x) \\
& =0
\end{aligned}
$$

The parameters $\lambda$ and $\mu$ are identified by developing the differential equation for the fast flux. The identification method leads to:

$$
\lambda^{2}+\mu^{2}=\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}} \quad \lambda^{2} \mu^{2}=\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}
$$

which gives a fourth-degree equation in $\lambda$ :

$$
\lambda^{4}-\lambda^{2}\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]+\left[\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}\right]=0
$$

for which the two solutions are:

$$
\begin{cases}\lambda_{\wedge}^{2}=\frac{\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]+\sqrt{\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]^{2}-4\left[\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}\right]}}{2} & >0 \\ \lambda_{\vee}{ }^{2}=\frac{\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]-\sqrt{\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]^{2}-4\left[\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}\right]}}{2} & >0\end{cases}
$$

If: $4\left[\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}\right]>\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]^{2}$
no solution in the real set exists. In practice, $L_{1 r}^{2} \approx 4 L_{2 r}^{2}$, i.e.:
$\left[\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}\right]^{2} \approx \frac{25}{16 L_{2 r}^{4}}$ and $4\left[\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}\right] \approx \frac{1}{L_{2 r}^{4}}$ by disregarding $\frac{1}{L_{U r}^{2} L_{R r}^{2}}$
Solutions in the set of real number thus exist. It be noted that the two solutions $\lambda_{\wedge}{ }^{2}$ and $\lambda_{\vee}{ }^{2}$ are positive and can be used later. Moreover, $\lambda_{\wedge}^{2}>\lambda_{\vee}^{2} \cdot \mu$ is evaluated using the equation:

$$
\left\{\begin{array}{l}
\mu_{\wedge}^{2}=\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}-\lambda_{\wedge}^{2}=\lambda_{\vee}{ }^{2}>0 \\
\mu_{\vee}^{2}=\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}-\lambda_{\vee}^{2}=\lambda_{\wedge}^{2}>0
\end{array}\right.
$$

It may be seen that here $\mu_{\wedge}^{2}<\mu_{\vee}^{2}$. The two possible solution couples $\left(\lambda_{\wedge}^{2}, \mu_{\wedge}^{2}\right)$ $\operatorname{and}\left(\lambda{ }^{2}, \mu_{\vee}^{2}\right)$ eventually result in a unique solution $\left(\lambda_{\wedge}^{2}, \lambda_{\vee}^{2}\right)$, for which the notation $\left(\lambda^{2}, \mu^{2}\right)$ is maintained to avoid any confusion. In the end, the fast flux that is zero at infinity can be expressed in the form:

$$
\Phi_{1 r}(x)=B e^{-\mu x}+D e^{-\lambda x}
$$

The thermal flux is calculated from the fast flux. Inserting the flux and current continuity conditions at the interface, we obtain:

$$
\left\{\begin{aligned}
\Phi_{1 r}(x) & =\left(\frac{\Phi_{1 r}(0)\left(\frac{L_{U r}^{2}}{L_{1 r}^{2}}-\lambda^{2} L_{U r}^{2}\right)-\Phi_{2 r}(0)}{\left(\mu^{2}-\lambda^{2}\right) L_{U r}^{2}}\right) e^{-\mu x}+\left(\frac{\Phi_{2 r}(0)-\Phi_{1 r}(0)\left(\frac{L_{U r}^{2}}{L_{1 r}^{2}}-\mu^{2} L_{U r}^{2}\right)}{\left(\mu^{2}-\lambda^{2}\right) L_{U r}^{2}}\right) e^{-\lambda x} \\
\Phi_{2 r}(x) & =\left(\frac{L_{U r}^{2}}{L_{1 r}^{2}}-\mu^{2} L_{U r}^{2}\right)\left(\frac{\Phi_{1 r}(0)\left(\frac{L_{U r}^{2}}{L_{1 r}^{2}}-\lambda^{2} L_{U r}^{2}\right)-\Phi_{2 r}(0)}{\left(\mu^{2}-\lambda^{2}\right) L_{U r}^{2}}\right) e^{-\mu x} \\
& +\left(\frac{L_{U r}^{2}}{L_{1 r}^{2}}-\lambda^{2} L_{U r}^{2}\right)\left(\frac{\Phi_{2 r}(0)-\Phi_{1 r}(0)\left(\frac{L_{U r}^{2}}{L_{1 r}^{2}}-\mu^{2} L_{U r}^{2}\right)}{\left(\mu^{2}-\lambda^{2}\right) L_{U r}^{2}}\right) e^{-\lambda x}
\end{aligned}\right.
$$

$\lambda$ and $\mu$ can be eliminated from the equation using the following formulae, which were seen earlier:

$$
\left\{\begin{array}{l}
\lambda^{2}+\mu^{2}=\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}} \quad \lambda^{2} \mu^{2}=\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}} \\
\lambda+\mu=\sqrt{(\lambda+\mu)^{2}}=\sqrt{\left(\lambda^{2}+\mu^{2}\right)+2 \lambda \mu}=\sqrt{\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}+2 \sqrt{\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}}} \\
\lambda \mu=\sqrt{\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}}
\end{array}\right.
$$

The fuel characteristic calculations are also straightforward:
Characteristics of the reflector:

$$
\left\{\begin{array}{c}
\frac{\frac{L_{U r}^{2}}{L_{1 r}^{2}}+L_{U r}^{2} \lambda \mu}{(\lambda+\mu)}-\frac{\Sigma_{2 \rightarrow 1, r}}{(\lambda+\mu)} \frac{\Phi_{2 r}(0)}{\Phi_{1 r}(0)}  \tag{13.27}\\
\frac{J_{2 r}(0)}{\Phi_{1 r}(0)}=\Sigma_{2 \rightarrow 1, r}(0)
\end{array} D_{2 r} L_{U r}^{2} \frac{\left(\frac{1}{L_{1 r}^{2}}-\mu^{2}\right)\left(\frac{1}{L_{1 r}^{2}}-\lambda^{2}\right)}{(\lambda+\mu)}+D_{2 r}\left(\frac{\left(\lambda^{2}+\mu^{2}+\lambda \mu\right)}{(\lambda+\mu)}-\frac{1}{L_{1 r}^{2}(\lambda+\mu)}\right) \frac{\Phi_{2 r}(0)}{\Phi_{1 r}(0)}\right.
$$

This leads back to the Lefebvre-Lebigot model since the up-scattering cross section $\Sigma_{\mathrm{Ur}}$ tends towards $0, \Sigma_{2 \rightarrow 1, r} L_{U r}^{2}=D_{1 r}$, and $1 / L_{U r 2}$ tends towards 0 . The term $\Sigma_{2 \rightarrow 1, r} / /(\lambda+\mu)$ also tends towards 0 due to $\Sigma_{2 \rightarrow 1, r}$.

Similarly, the term $\Sigma_{2 \rightarrow 1, r}\left(L_{U r}^{2} / L_{1 r}^{2}+L_{U r}^{2} \lambda \mu\right) /(\lambda+\mu)$ tends towards $D_{1 r} / L_{1 r}$. Given that:

$$
\begin{aligned}
& -D_{2 r} L_{U r}^{2}\left(\frac{1}{L_{1 r}^{2}}-\mu^{2}\right)\left(\frac{1}{L_{1 r}^{2}}-\lambda^{2}\right) \\
& =-D_{2 r} L_{U r}^{2}\left(\begin{array}{c}
\frac{1}{L_{1 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{1 r}^{2}} \underbrace{\frac{1}{L_{1 r}^{2}}+\frac{1}{L_{2 r}^{2}}}_{\frac{1}{\left(\lambda^{2}+\mu^{2}\right)}}+\underbrace{\lambda^{2}}_{\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U}^{2} L_{R r}^{2}}}
\end{array}\right)=\frac{D_{2 r}}{L_{R r}^{2}}=\Sigma_{1 \rightarrow 2, r}
\end{aligned}
$$

the transfer matrix $\mathfrak{R}$ of the Poincaré-Steklov operator at the interface relates the neutron current to the flux as expressed:
$\mathfrak{R}=\left(\begin{array}{cc}\frac{\frac{1}{L_{1 r}^{2}}+\sqrt{\frac{1}{L_{2 r}^{2} L_{1 r}^{2}}-\frac{1}{L_{U r}^{2} L_{R r}^{2}}}}{(\lambda+\mu)} & -\frac{\Sigma_{2 \rightarrow 1, r}}{(\lambda+\mu)} \\ D_{1 r} & D_{2 r}\left(\frac{\Sigma_{1 \rightarrow 2, r}}{(\lambda+\mu)}\right.\end{array}\right)$
The infinite albedo matrix $\left(\beta_{i j}\right)^{\infty}$ is also obtained by expressing the outgoing currents with respect to the incoming currents (Fig. 13.19):

$$
\begin{aligned}
\binom{J_{1}^{-}}{J_{2}^{-}}= & \binom{\frac{\left(\frac{1}{2}+\Re_{22}\right)\left(\frac{1}{2}-\Re_{11}\right)+\Re_{12} \Re_{21}}{\left(\frac{1}{2}+\Re_{22}\right)\left(\frac{1}{2}+\Re_{11}\right)-\Re_{12} \Re_{21}}-\frac{\Re_{12}}{\left(\frac{1}{2}+\Re_{22}\right)\left(\frac{1}{2}+\Re_{11}\right)-\Re_{12} \Re_{21}}}{-\frac{\mathfrak{R}_{21}}{\left(\frac{1}{2}+\Re_{22}\right)\left(\frac{1}{2}+\Re_{11}\right)-\Re_{12} \Re_{21}} \frac{\left(\frac{1}{2}+\Re_{11}\right)\left(\frac{1}{2}-\Re_{22}\right)+\Re_{21} \Re_{12}}{\left(\frac{1}{2}+\Re_{22}\right)\left(\frac{1}{2}+\Re_{11}\right)-\Re_{12} \Re_{21}}} \\
& \times\left(\begin{array}{l}
J_{1}{ }^{+} \\
\left.J_{2}{ }^{+}\right)
\end{array}\right.
\end{aligned}
$$

The difference with respect to the Lefebvre-Lebigot model without up-scattering is that the fast characteristic is a linearly decreasing function. An additional unknown has been added to the system (the up-scattering cross section), thereby leading to six unknowns. Four coefficients still need to be evaluated. As previously, two degrees of freedom remain. In the model without up-scattering, the absolute error on the ratio $J_{1} / \Phi_{1}$ was around $1 \%$. Allowing for up-scattering reduces this


Fig. 13.19 Graphical view of the operating point with up-scattering
error to $0.1 \%$. On the other hand, for the ratio $J_{2} / \Phi_{1}$, the error is still under $0.4 \%$ in both models. As a reminder, the up-scattering term appears only in the fast flux equation. Finally, it should be pointed out that the values of 1.3 and 0.4 for the fast and thermal diffusion coefficients of the reflector being set, the identification for the other cross section values leads to a negative up-scattering cross section $\Sigma_{2 \rightarrow 1, r}$, i.e. $L_{U r 2}$ is also negative (despite the square operation). This result is very surprising, and must be analyzed only in the framework of a mathematical reflector which does not truly represent the scattering of neutrons, but simply provides an "equivalent" effect to a true reflector at the interface.

The Lefebvre-Lebigot model has been employed in the official EDF calculation chain, and has proved to be extremely robust for all the different fuel management schemes and reactor types. It is very simple to set up in a calculation scheme and provides a fitting parameter for the measured flux distributions with only the fast diffusion coefficient. Comparisons with more complex models (in particular, the generalized beta model which will be discussed below) showed that it was precise enough for industrial applications. Only accidental cases with a high void fraction in the reflector can challenge this conclusion given that the conditions are very different from its validity range.

### 13.10 Diffusion/Transport Correspondence

We have just illustrated the modeling of a reflector in two energy-group diffusion theory with up-scattering. If the driver zone is modeled with transport theory such as the $S_{n}$ method or in simplified transport with $S P_{n}$-especially for the $S P_{1}$ case, the following corresponding terms (the term equivalence is not used here, as transport-diffusion equivalence has a very specific meaning in neutron physics) are used:

$$
\left\{\begin{array}{l}
D_{1 r}=\frac{1}{3 \Sigma_{\text {transport } 1, r}}=\frac{1}{3\left(\Sigma_{t 1, r}-\sum_{g^{\prime}} \Sigma_{s_{1}}^{1 \rightarrow g^{\prime}}\right)}=\frac{1}{3\left(\Sigma_{t_{1} r}-\Sigma_{s_{1} r}^{(1)}\right)} \\
D_{2 r}=\frac{1}{3 \Sigma_{\text {transport } 2, r}}=\frac{1}{3\left(\Sigma_{t 2, r}-\sum_{g^{\prime}} \Sigma_{s_{1}}^{2 \rightarrow g^{\prime}}\right)}=\frac{1}{3\left(\Sigma_{t_{2} r}-\Sigma_{s_{1} r}^{(2)}\right)} \\
\Sigma_{t 1, r}=\Sigma_{a 1, r}+\Sigma_{1 \rightarrow 2, r}+\Sigma_{1 \rightarrow 1, r} \quad \Sigma_{t 2, r}=\Sigma_{a 2, r}+\Sigma_{2 \rightarrow 1, r}+\Sigma_{2 \rightarrow 2, r}
\end{array}\right.
$$

The $S P_{1}$ method can be employed to obtain an equivalent solution to the diffusion method by adapting the diffusion coefficient.

### 13.11 Reuss-Nisan Model

The Reuss-Nisan ${ }^{12}$ reflector model was conceived at the $C E A$ in the 1970s to model the core/baffle/reflector interface with an equivalent reflector in multi-group diffusion. The baffle is a steel structure in the form of sheets that surrounds the perimeter of the active core in $P W R$. The principle is to compute the albedo matrix of the baffle of thickness $e$ and that of the reflector assumed to be infinite, so as to determine the equivalent matrix for both materials. This problem is somewhat simplified by assuming that there is no up-scattering between the $G$ energy groups, thereby implying that there is only one thermal group. In this approximation, the albedo matrix has lower triangular shape and there are $G(G+1) / 2$ matrix elements to calculate (Picture 13.2).

The $G$ diffusion equations in the reflector are written as:
Multi-group diffusion equation in the reflector:

$$
\begin{equation*}
-D_{g} \Delta \Phi_{g}(x)+\Sigma_{t, g} \Phi_{g}(x)=\sum_{g^{\prime}<g} \Sigma_{g^{\prime} \rightarrow g} \Phi_{g^{\prime}}(x) \quad g=1, \ldots, G \tag{13.28}
\end{equation*}
$$

The differential scattering cross section $\Sigma_{g}{ }^{\prime} \rightarrow g$ is sometimes denoted as $\Sigma_{g g}$ to obtain a lower triangular matrix since $\Sigma_{g}, \rightarrow g=0$ when $g^{\prime}>g$, as the fastest energy group is usually numbered 1 , with the index increasing as the neutron is thermalized. The notation $\Sigma_{g}, g$ leads to an upper triangular matrix. The first notation is preferred since it is entirely unambiguous. The general solution to the homogeneous equation is given by:

[^279]

Picture 13.2 Paul Reuss (1940-) conceived several neutron models during his career at the CEA after his studies at Ecole Polytechnique (1960-1962). He later obtained a PhD in 1979 on the "effect of plutonium recycling in water-moderated reactors". He is also famous for having published more than ten books on neutron physics and nuclear energy in general, for which he proved to be an excellent and may be the best popularizer in France (Courtesy Reuss).

$$
\Phi_{g}(x)=\alpha_{g} e^{+\kappa_{g} x}+\delta_{g} e^{-\kappa_{g} x}
$$

with: $\kappa_{g}=\sqrt{\frac{\Sigma_{t, g}}{D_{g}}}$
The particular solution for the inhomogeneous equation is expressed as:

$$
\Phi_{g}(x)=\sum_{k<g} \gamma_{g k}\left(\alpha_{k} e^{+\kappa_{k} x}+\delta_{k} e^{-\kappa_{k} x}\right)
$$

The notation $\gamma_{g k}$ (instead of $\gamma_{k g}$ ) keeps a lower triangular matrix. Inserting this term in the differential equation leads to:

$$
\begin{aligned}
& \sum_{k<g}-\gamma_{g k}\left(\alpha_{k} \kappa_{k}^{2} e^{+\kappa_{k} x}+\delta_{k} \kappa_{k}^{2} e^{-\kappa_{k} x}\right)+\kappa_{g}^{2} \sum_{k<g} \gamma_{g k}\left(\alpha_{k} e^{+\kappa_{k} x}+\delta_{k} e^{-\kappa_{k} x}\right) \\
& \quad=\sum_{i<g} \frac{\Sigma_{i \rightarrow g}}{D_{g}} \sum_{h<i} \gamma_{i h}\left(\alpha_{h} e^{+\kappa_{h} x}+\delta_{h} e^{-\kappa_{h} x}\right)
\end{aligned}
$$

The similar positive or negative exponential terms are grouped together, hence:

$$
\left\{\begin{array}{l}
\sum_{k<g} \gamma_{g k} \alpha_{k}\left(\kappa_{k}^{2}-\kappa_{g}^{2}\right) e^{+\kappa_{k} x}=\sum_{i<g} \frac{\Sigma_{i \rightarrow g}}{D_{g}} \sum_{h<i} \gamma_{i h} \alpha_{h} e^{+\kappa_{h} x} \\
\sum_{k<g} \gamma_{g k} \delta_{k}\left(\kappa_{k}^{2}-\kappa_{g}^{2}\right) e^{-\kappa_{k} x}=\sum_{i<g} \frac{\Sigma_{i \rightarrow g}}{D_{g}} \sum_{h<i} \gamma_{i h} \delta_{h} e^{-\kappa_{h} x}
\end{array}\right.
$$

The exponentials form a basis set, and thus, the coefficients for similar exponential terms can be determined by direct term identification, with $k=h=m$ :

$$
\left\{\begin{array}{l}
\gamma_{g m} \alpha_{m}\left(\kappa_{m}^{2}-\kappa_{g}^{2}\right) e^{+\kappa_{m} x}=\sum_{i<g} \frac{\Sigma_{i \rightarrow g}}{D_{g}} \gamma_{i m} \alpha_{m} e^{+\kappa_{m} x} \\
\gamma_{m g} \delta_{g m}\left(\kappa_{m}^{2}-\kappa_{g}^{2}\right) e^{-\kappa_{m} x}=\sum_{i<g} \frac{\Sigma_{i \rightarrow g}}{D_{g}} \gamma_{i m} \delta_{m} e^{-\kappa_{m} x}
\end{array}\right.
$$

These equations are similar for the $\alpha_{m}$ or $\beta_{m}$ terms. Therefore, the recurrence relations for the coefficients $\gamma_{m g}$ can be deduced as:

Recurrence relation for the coefficients of the flux in the reflector:

$$
\begin{equation*}
\gamma_{g m}=\frac{1}{D_{g}\left(\kappa_{m}^{2}-\kappa_{g}^{2}\right)} \sum_{i<g} \Sigma_{i \rightarrow g} \gamma_{i m} \tag{13.29}
\end{equation*}
$$

The first term of the recurrence is obtained by setting $m=g$ and recalling that $\Sigma_{i g}=0$ for $i>g$. In fact, $\gamma_{g g}$ is the coefficient for the solution of the homogeneous equation, i.e. 1. Thus:

$$
\left\{\begin{array}{cl}
\gamma_{g m}=0 & \text { for } m>g \\
\gamma_{g g}=1 & \text { for } m<g
\end{array}\right.
$$

The general solution is the sum of the particular and general solutions for the homogeneous equation:

$$
\Phi_{g}(x)=\alpha_{g} e^{+\kappa_{g} x}+\beta_{g} e^{-\kappa_{g} x}+\sum_{k<g} \gamma_{g k}\left(\alpha_{k} e^{+\kappa_{k} x}+{ }_{k} e^{-\kappa_{k} x}\right)
$$

and by including the general solution in the summation operator using $\gamma_{g g}=1$ :
Multi-group flux without up-scattering:

$$
\begin{equation*}
\Phi_{g}(x)=\sum_{k \leq g} \gamma_{g k}\left(\alpha_{k} e^{+\kappa_{k} x}+\delta_{k} e^{-\kappa_{k} x}\right) \tag{13.30}
\end{equation*}
$$

The albedo matrix relates the negative currents to the positive currents of the core/reflector interface by:

$$
J_{g}^{-}=\sum_{i} \beta_{j i} J_{i}^{+}=\sum_{i \leq j} \beta_{j i} J_{i}^{+}
$$

since the albedo matrix is lower triangular. In diffusion theory, the incoming and outgoing currents are given by:

$$
J_{g}^{+}(x)=\frac{\Phi_{g}(x)}{4}-\frac{D_{g}}{2} \frac{d \Phi_{g}(x)}{d x} \text { and } J_{g}^{-}(x)=\frac{\Phi_{g}(x)}{4}+\frac{D_{g}}{2} \frac{d \Phi_{g}(x)}{d x}
$$

i.e.:

$$
\left\{\begin{array}{l}
J_{g}^{+}(x)=\sum_{k \leq g} \gamma_{g k}\left[\frac{\alpha_{k}}{4}\left(1-2 D_{g} \kappa_{k}\right) e^{+\kappa_{k} x}+\frac{\beta_{k}}{4}\left(1+2 D_{g} \kappa_{k}\right) e^{-\kappa_{k} x}\right] \\
J_{g}^{-}(x)=\sum_{k \leq g} \gamma_{g k}\left[\frac{\alpha_{k}}{4}\left(1+2 D_{g} \kappa_{k}\right) e^{+\kappa_{k} x}+\frac{\beta_{k}}{4}\left(1-2 D_{g} \kappa_{k}\right) e^{-\kappa_{k} x}\right]
\end{array}\right.
$$

It should be noted that if the reflector is infinite, the $\alpha_{k}$ coefficients must all be zero for the flux and currents to have finite values. To obtain the elements of the albedo matrix, it is assumed that:

- only one group current is non zero, i.e. $J_{g}^{+}(0)=1$,
- the currents in the other groups are equal to zero.

Thus, there is a vector of $G$ elements such that:
$\{0,0,0, \ldots 0, \underbrace{1}_{J_{s}^{+}}, 0, \ldots 0\}$ corresponds to the hypothetical case for $g$
For this hypothetical case (there is a total of $G$ cases), the following equation is reached:

$$
\beta_{g g^{\prime}}=J_{g}^{-}(0) \quad \text { computed for the hypothetical case } g^{\prime}
$$

Since $J_{g}^{-}(0)=\sum_{k \leq g} \gamma_{g k} \frac{\delta_{k}}{4}\left(1-2 D_{g} \kappa_{k}\right)$, the unknowns are the $G$ values of $\left(\delta_{k}\right)_{\text {case } g^{\prime}}$ obtained by expressing the linear system of $G$ equations, defined by the conditions on $J_{g}^{+}(0)$ :

Outgoing current at the core/reflector interface:

$$
\begin{cases}J_{g}^{+}(0)=\sum_{k \leq g} \gamma_{g k} \frac{\delta_{k}}{4}\left(1-2 D_{g} \kappa_{k}\right)=0 & \text { for } g \neq g^{\prime}  \tag{13.31}\\ J_{g^{\prime}}^{+}(0)=\sum_{k \leq g^{\prime}} \gamma_{g^{\prime} k} \frac{\delta_{k}}{4}\left(1-2 D_{g^{\prime}} \kappa_{k}\right)=1 & \text { for } g=g^{\prime}\end{cases}
$$

Solving the $G$-equation system for each hypothetical case leads to the $G(G+1) / 2$ albedo values $\beta_{g g^{\prime}}$ for the infinite homogeneous reflector without baffle (Figs. 13.20 and 13.21).

Allowance for the baffle surrounding the core perimeter is derived from the previous calculations. Given that $e$ is the baffle thickness, the incoming and outgoing currents at both interfaces for $G$ groups are:

Incoming current at the core/reflector interface:

$$
\left\{\begin{array}{l}
J_{g}^{-}(0)=\sum_{k \leq g} \theta_{g k} J_{k}^{+}(0)+\tau_{g k} J_{k}^{-}(e)  \tag{13.32}\\
J_{g}^{+}(e)=\sum_{k \leq g} \theta_{g k} J_{k}^{-}(e)+\tau_{g k} J_{k}^{+}(0)
\end{array} \text { for g from 1 to } G\right.
$$

The coefficients $\theta_{g k}$ and $\tau_{g k}$ are determined by hypothetical cases where only $J_{g^{\prime}}^{+}(0)=1$ and $J_{g^{\prime}}^{-}(e)=0$, thereby leading to the hypothetical condition:

Fig. 13.20 Core/infinite reflector interface


Fig. 13.21 Core/infinite reflector interface


$$
\left\{\begin{array}{l}
\theta_{g g^{\prime}}=J_{g}^{-}(0)_{\text {situation }} g^{\prime} \\
\tau_{g g^{\prime}}=J_{g}^{+}(e)_{\text {situation }} g^{\prime}
\end{array}\right.
$$

It should be carefully noted that the positive exponential terms are retained in the flux calculation for the baffle since the latter is finite, thus:

$$
\left\{\begin{array}{c}
J_{g}^{-}(0)=\sum_{k \leq g} \gamma_{g k}\left[\frac{\alpha_{k}}{4}\left(1+2 D_{g} \kappa_{k}\right)+\frac{\delta_{k}}{4}\left(1-2 D_{g} \kappa_{k}\right)\right] \\
J_{g}^{+}(e)=\sum_{k \leq g} \gamma_{g k}\left[\frac{\alpha_{k}}{4}\left(1+2 D_{g} \kappa_{k}\right) e^{+\kappa_{k} e}+\frac{\delta_{k}}{4}\left(1-2 D_{g} \kappa_{k}\right) e^{-\kappa_{k} e}\right]
\end{array} \text { for g from 1 to } G\right.
$$

The solution of the $G$ systems with $2 G$ equations for hypothetical cases is used to evaluate the $2 G$ series of coefficients $\left(\alpha_{k}\right)_{\text {case } g^{\prime}}$ and $\left(\delta_{k}\right)_{\text {case } g^{\prime}}$. The currents at the baffle/reflector interface may now be computed by also introducing the reflector albedo $\beta_{g k}$ :

$$
\left\{\begin{array}{c}
J_{g}^{+}(e)=\sum_{k \leq g} \theta_{g k} J_{k}^{-}(e)+\tau_{g k} J_{k}^{+}(0) \\
J_{g}^{-}(e)=\sum_{k \leq g} \beta_{g k} J_{k}^{+}(e)
\end{array}\right.
$$

The outgoing current from the core/baffle interface is given by a third equation:
Incoming current at the core/baffle interface:

$$
\begin{equation*}
J_{g}^{-}(0)=\sum_{k \leq g} \theta_{g k} J_{k}^{+}(0)+\tau_{g k} J_{k}^{-}(e) \tag{13.33}
\end{equation*}
$$

Once again, $G$ hypothetical cases are employed with $J_{g^{\prime}}^{+}(0)=1$, and the other incoming currents are zero, resulting in $G$ currents $J_{g^{\prime}}^{-}(e)$ and $J_{g^{\prime}}^{+}(e)$, that are further used to evaluate $J_{g}^{-}(0)$. The equivalent reflector that integrates a unique response for both the baffle and the reflector, satisfies:

$$
J_{g}^{-}(0)=\sum_{k \leq g} \beta_{g k}^{\text {equivalent }} J_{g}^{+}(0)
$$

such that the currents $J_{g}^{-}(0)$ and $J_{g}^{+}(0)$ for the core/baffle/reflector calculation are conserved. As previously:

$$
\beta_{g g^{\prime}}^{\text {equivalent }}=J_{g}^{-}(0) \quad \text { for the case } g^{\prime} \text { where } \quad J_{g^{\prime}}^{+}(0)=1
$$

Knowing the albedo matrix of the equivalent reflector, and if the diffusion coefficients are set, the cross sections and the attenuation coefficients $\kappa_{g}$ of the
decreasing exponential can be computed by recurrence on the energy groups. If applied to a two energy group problem without up-scattering, three coefficients are calculated for the albedo matrix of the equivalent reflector ( $\beta_{12}^{\text {equivalent }}=0$ ). The albedo values depend on five parameters: $D_{1}, D_{2}, \Sigma_{a 1}, \Sigma_{a 2}$ and $\Sigma_{1 \rightarrow 2}$. Hence, just like for the Lefebvre-Lebigot method, there are two degrees of freedom. In this case, the authors decided to conserve the diffusion coefficients in the baffle. The calculations are carried out in three steps:

- The diffusion coefficients of the baffle and moderator are computed in infinite homogeneous lattice approximation with a core/baffle and core/water (pseudo-) infinite slab geometries.
- Afterwards, a slab geometry with core/baffle/water is computed with the core being a homogeneous medium corresponding to an assembly at the core periphery. For each medium, the neutron quantities $\Sigma_{a 1}, \Sigma_{a 2}$ and $\Sigma_{1 \rightarrow 2}$ are evaluated.
- Finally, the true reflector is substituted by the equivalent reflector with a diffusion/diffusion calculation described previously, by computing the albedo of the equivalent reflector in terms of albedo matrices and baffle transmission.

As for the Lefebvre-Lebigot model, this model is a $1 D$ representation of the core/ reflector slabs and does not model the $2 D$ geometry of a true baffle. Hence, the validity of this model for the incoming and outgoing corners of the core may legitimately be questioned.

### 13.12 Mondot Model

Jacques Mondot ${ }^{13}$ proposed a method to conserve the multi-group albedo at the interface. Let us consider a homogeneous reflector defined by neutron constants $D_{g}$, $\Sigma_{T g}$ and $\Sigma_{g}{ }^{\prime} \rightarrow g$. The albedo condition at the core/reflector interface is given by the matrix equation:

$$
J^{+}(0)=\beta J^{-}(0)
$$

where $J^{+}(0)$ is the outgoing current from the reflector and $J^{-}(0)$ the incoming current (N.B. These currents are not given with respect to the core, as is normally the case) (Fig. 13.22).

[^280]Fig. 13.22 Core/infinite reflector interface (Mondot model)


The currents are expressed by the usual relations, while being careful with the + and - signs due to the conventions employed:

$$
J^{-}(0)=\frac{\Phi(0)}{4}+\frac{J(0)}{2} \text { and } J^{+}(0)=\frac{\Phi(0)}{4}-\frac{J(0)}{2}
$$

The net current is related to the flux through the transfer matrix:

$$
J(0)=\Re \Phi(0)
$$

Thus, $\mathfrak{R}$ can be calculated as a function of the albedo matrix $\beta$ :

$$
\left\{\begin{array}{l}
J^{-}(0)=\frac{\Phi(0)}{4}+\frac{\mathfrak{R} \Phi(0)}{2}=\frac{\Phi(0)}{2}\left(\frac{1}{2} I+\mathfrak{R}\right) \\
J^{+}(0)=\frac{\Phi(0)}{4}-\frac{\mathfrak{R} \Phi(0)}{2}=\frac{\Phi(0)}{2}\left(\frac{1}{2} I-\Re\right)
\end{array}\right.
$$

Hence: $\mathfrak{R}=\frac{1}{2}(1-\beta)(1+\beta)^{-1}$
The multi-group diffusion equation is expressed in matrix form as:

$$
-\mathrm{D} \Delta \Phi+\Sigma \Phi=0
$$

where $\mathrm{D}=\left[D_{g}\right]$ is a diagonal matrix, $\Sigma$ is a lower triangular matrix when there is no up-scattering, and $\Phi=\left[\Phi_{g}\right]$ and $\Delta \Phi=\left[\Delta \Phi_{g}\right]$ are also diagonal matrices. For the associated homogeneous equation:

$$
\Delta \Phi_{0}-\mathrm{K}^{2} \Phi_{0}=0
$$

where $\mathrm{K}^{2}$ is the diagonal matrix with $\kappa_{g}^{2}=\Sigma_{T g} / D_{g}$ terms. The solution to this equation in slab geometry with null flux at infinity is given by:

$$
\Phi_{0}=\left[\begin{array}{ll}
C_{g} & e^{-\kappa_{g} x}
\end{array}\right]
$$

The general solution to the diffusion equation is written as follows in matrix form:

$$
\Phi=\mathrm{A} \Phi_{0}
$$

This expression is inserted in the diffusion equation, thereby resulting in:

$$
\begin{align*}
& -\mathrm{DA} \Delta \Phi_{0}+\Sigma \Phi=-\mathrm{DAK}^{2} \Phi_{0}+\Sigma A \Phi_{0}=0 \\
& \text { Or }: \mathrm{D}^{-1} \Sigma A=\mathrm{AK}^{2} \tag{13.34}
\end{align*}
$$

It follows that A is the matrix that is the eigenvector of $\mathrm{D}^{-1} \Sigma$, and that $\mathrm{K}^{2}$ is the matrix of eigenvalues. At the interface $(x=0), \Phi(0)=\mathrm{A} \Phi_{0}(0)=\mathrm{A}\left\lfloor C_{g}\right\rfloor$, thus:

$$
\mathrm{J}(0)=-\mathrm{D} \nabla \Phi(0)=\mathrm{D} A \mathrm{~K} \mathrm{C}=\mathrm{DA} \mathrm{~K} \mathrm{~A}^{-1} \Phi(0)=\Re \Phi(0)
$$

We deduce that: $\mathfrak{R}=\mathrm{D}$ A K $\mathrm{A}^{-1}$
From Eq. (13.34), $\Sigma=\mathrm{DAK}^{2} \mathrm{~A}^{-1}$, therefore:

$$
\begin{equation*}
\Sigma=\mathrm{D} \mathrm{~A}^{2} \mathrm{~A}^{-1}=\mathfrak{R} \mathrm{D}^{-1} \mathfrak{R} \tag{13.35}
\end{equation*}
$$

D and $\Sigma$ cannot be calculated simultaneously. However, if D is imposed, the matrix $\Sigma$ can be determined such that the albedo conditions are satisfied. There are $G(G+1) / 2$ known albedo values, $G(G+1) / 2$ cross section values ( $\Sigma$ is a lower triangular matrix), and $G$ diffusion coefficient values ( D is a diagonal matrix). Hence, there are $G$ degrees of freedom. At this point, the values of D can be chosen arbitrarily. The Reuss-Nisan method recommends using the values for the baffle diffusion coefficients, while the Lefebvre-Lebigot model recommends those of the fuel zone. Mondot recommends an equivalence between the transport and the homogeneous diffusion calculations using the same spatial mesh (coarse mesh). Iterations are performed until the albedo values at the interface converge. The Mondot method can only be applied for albedos in multi-group diffusion theory without up-scattering. In the 1990s, the CEA generalized this method for other methods, removing the limitations due to up-scattering for a wider application: this method is called the generalized BETA method.

### 13.13 Generalized BETA Method

The generalized BETA ${ }^{14}$ method consists in calculating the neutron quantities of the reflector by imposing a neutron source at the interface of the reflector medium for a departure energy group (Fig. 13.23).

[^281]Fig. 13.23 Core/infinite reflector interface (generalized BETA model)


The following equation is solved for one departure energy group:

$$
H_{g} \Phi_{n+1}^{g}=S_{g}^{n}
$$

where:
$S_{g}^{n}=\left\{\delta_{1 g}, \delta_{2 g}, \ldots, \delta_{G g}\right\}$ is a unit source in the given energy group
$H_{g}$ is the operator for the core code under consideration (diffusion or transport)
$\Phi_{n+1}^{g}$ is the flux response to the unit source
The reference albedo values to be retained are those computed by a Monte Carlo code (TRIPOLI) so as to correctly evaluate the anisotropy due to iron. There are as many Monte Carlo calculations as the number of energy groups. As for the foregoing methods, let us consider that there are $G$ degrees of freedom, assuming that there are $G^{2}$ albedo values. We must calculate $G$ diffusion coefficients and $G^{2}$ differential scattering cross sections (assuming that up-scattering is possible for all energy groups). The authors chose to conserve the total cross section $\Sigma_{t, g}$. In diffusion theory, the diffusion coefficient and the differential cross section are corrected with a fixed removal cross section until convergence towards the reference albedo. In transport theory, the total cross section is corrected by means of differential scattering cross sections (within-group or self-scattering), such that the total removal cross section remains unchanged. The off-diagonal differential cross sections are also corrected using the fixed removal cross section. This method, despite being more general, has not been extensively validated on industrial cores.

### 13.14 Absorption in the Reflector

Through a $1 D$ slab calculation of the radial reflector for a $C P Y(900 \mathrm{MWe})$, the rise of the thermal flux (cut-off at 0.625 eV ) in the successive steel layers of the reflector (baffle/barrel/thermal shield/vessel) can be plotted (Fig. 13.24). The core/reflector interface is represented by the red vertical line. The fuel is assumed to be homogeneous ( $3.7 \%$ enrichment in ${ }^{235} U$ at a burn-up of $150 \mathrm{MWd} /$ ton). The fluxes are normalized to 1 emitted neutron per second. It can be seen that the thermal absorption is very weak in the regions comprising water only. However, it increases in regions that include steel. After 40 cm of reflector, the fluxes tend towards 0 with an exponential decay.

Fig. 13.24 Reflector physics for a $P W R$



### 13.15 Double-Differential Albedo

(Shultis and Faw 2000, p. 236)
The most general definition of an albedo for a material is the ratio of the emitted radiation to the incident radiation, whether the radiation comprises a beam of neutrons or $\gamma$ rays (Figs. 13.25 and 13.26). If $J\left(E_{i}, \theta_{i}\right)$ is the incident radiation

Fig. 13.25 Definition of angles that appear in the double-differential albedo


Fig. 13.26 "True" path of a neutron in matter

current at energy $E_{i}$ and $\theta_{i}$ the angle with respect to the normal x, and $J\left(E_{o}, \theta_{o}, \phi_{o}\right)$ is the outgoing current at energy $E_{o}$ (usually with energy loss), with a polar angle $\theta_{o}$ and an azimuthal angle $\varphi_{o}$, the double-differential albedo is defined as the ratio of the incoming and outgoing currents:

$$
\beta\left(E_{i} \rightarrow E_{o}, \theta_{i} \rightarrow \theta_{o}, \varphi_{o}\right)=\frac{J\left(E_{o}, \theta_{o}, \varphi_{o}\right)}{J\left(E_{i}, \theta_{i}\right)}
$$

The double-differential albedo represents the complex phenomenon of the path of a neutron that enters matter and scatters within it to get out at any angle with a different energy. The advantage of using such albedos is that the reflection of a given radiation on a surface can be modeled without the need for calculation of interactions inside the materials themselves. In a radiation transport problem, this implies significant savings in calculation time, and several applications in radiation shielding can be considered. ${ }^{15}$ We have seen that the albedo of neutrons can be modeled using simple functions since the angular distribution of reflected neutrons does not depend on the azimuthal angle $\varphi_{o}$ and has the general shape of a cosine function of the reflection angle $\theta_{o}$.

Hence, for thermal neutrons, the law of Eq. (13.36) correctly represents the distribution of reflected incident thermal neutrons:

[^282]Table 13.4 Reflection albedo for concrete and iron (Christian Devillers, Pierre Lafore: Réacteurs à caisson de pression en béton précontraint [Reactors with pre-stressed concrete chambers], technical report CEA-N 504, 1965)

|  | Ordinary concrete | Iron |
| :--- | :--- | :--- |
| Neutrons at $2200 \mathrm{~m} / \mathrm{s}$ | $\frac{1}{0.297 \cos \theta_{I}+1,33} \frac{\cos \theta_{O}}{\pi}$ | $\frac{1}{1.48 \cos \theta_{I}+1,88} \frac{\cos \theta_{O}}{\pi}$ |
| Dose current albedo (neutrons at 2 MeV ) | $\frac{0.334}{\left[\cos \theta_{l}\right]^{0.333}} \frac{\cos \theta_{O}}{\pi}$ | $\frac{1}{1.07 \cos \theta_{l}+1.43} \frac{\cos \theta_{O}}{\pi}$ |

Differential albedos of thermal neutrons:

$$
\begin{equation*}
\beta\left(\theta_{I}, \theta_{O}\right)=\frac{1}{a \cos \theta_{I}+b} \frac{\cos \theta_{O}}{\pi} \tag{13.36}
\end{equation*}
$$

For fast neutrons, the albedo corresponding to a given cross section $\Sigma$ (scattering, dose, etc.) can be defined, either in the form of Eq. (13.36), or as:

Differential albedos of fast neutrons: $\quad \beta\left(\theta_{I}, \theta_{O}\right)=\frac{a}{\cos ^{n} \theta_{I}} \frac{\cos \theta_{O}}{\pi}$
These formulations are less valid for grazing incident angles, for which dependence on the azimuthal angle must be taken into account. Furthermore, the distribution of reflected neutrons has peaks for some values of $\cos \theta_{O}$. For instance, the albedos for thermal and fast neutrons (dose cross-sections) for concrete and iron are given in (Table 13.4).

The use of surface albedos leads to a problem that can be modeled by an optical approach of neutron reflection by surfaces, via transmission factors that are applicable to neutron guides (tubes in structural elements, etc.) (Squires 1996, p. 11).

## Chapter 14 <br> Heterogeneous Reactors

Industrial reactors have complex geometries, with the nuclear fuel being geometrically separated from the coolant. Furthermore, different materials are used to allow for mechanical and thermal stresses due to the emitted energy. Hence, the homogeneous model cannot be applied in all situations, which leads to more complex neutron models for calculations.
(Meghreblian and Holmes 1960, p. 626)

### 14.1 Why Is Heterogeneity Desirable?

At this point, it is clear that a homogeneous reactor is the simplest case to calculate. However, it is not exactly representative of either neutron physics or the technology employed in energy production. During its lifetime in the reactor, a neutron is slowed down, reaching epithermal energy where several resonances are present, especially those of ${ }_{92}^{238} U$, which are abundantly present in the reactor. Slowing-down in the resonance zone is a critical phase during which almost $30 \%$ of neutrons do not "survive" (the resonance escape probability is about 0.7). If a homogeneous reactor is considered with a homogeneous solution of fissile nuclides and moderator, the continuous slowing-down process by collision with the moderator increases the chances of the neutron being captured in resonances. Separating the moderator from the fuel increases the probabilities that neutrons emitted from the fuel then slowed down by the moderator will escape resonant capture (Marchuk 1959, p. 167). The reference work, (Kahan and Gauzit 1957), illustrates this effect by showing the impact of the ratio of concentrations of graphite to natural uranium in moles on the $k_{\infty}$ of a homogeneous solution (Fig. 14.1).

An optimum moderation ratio of $N_{\text {graphite }} / N_{\text {Uranium }}=400$ is obtained, i.e. $k_{\infty}^{\max }=0.8$. Already in 1942, Enrico Fermi was conscious that for a maximum $f p$ of just 0.6 , the infinite multiplication factor $k_{\infty}$ of a homogeneous reactor with natural


| $\qquad$ Resonance escape probability $p$ |  |
| :---: | :---: |
| $\qquad$ |  |
| k ${ }^{\circ}$ |  |
|  | Neutron per absorption |
| - $\varepsilon$ |  |

Fig. 14.1 Reactivity effect of the moderation ratio of a homogeneous solution of natural uranium and graphite [after (Kahan and Gauzit 1957)]


Fig. 14.2 Heterogeneous lattice of fuel pins
$\operatorname{uranium}(\eta=1.33$ and $\varepsilon=1.05)$ mixed with graphite would not be more than 0.85 . In particular, it should be noted that such a homogeneous reactor cannot become critical with natural uranium (Blanc 1986, p. 52). A heterogeneous lattice of uranium pins in a pile of graphite leads to criticality. In 1942, the principle of separating the nuclear fuel from the moderator led Alvin Weinberg (1915-2006) and Eugen Wigner to propose the cooling of uranium oxide at the same time as the moderation of neutrons using light water rather than carbon. The neutrons are mostly slowed down in water and escape capture, and thus return to the fuel pins with an energy at which fission is possible. Indeed, the lattice size (its pitch) and the fuel geometry have a significant impact on the achievable multiplication factor (Fig. 14.2).

From a technological point of view, the goal is to transfer heat from the fuel to a moving coolant, leading quite naturally to a geometrical separation of the fuel from the moderating fluid. Molten salt reactors, on the other hand, do not operate according to this principle. These reactors in fact utilize a homogeneous liquid fuel and the fuel motion itself drains heat out of the core to the exchanger. However, in fast neutron reactors, neutron energy is conserved as far as possible in order to avoid resonant capture, and to harness the fission of ${ }_{92}^{238} U$, thus excluding the use of
moderating materials. Finally, the fuel is enclosed in a cladding that acts as an initial protective barrier to avoid the dissemination of radioactive products created by fission. From the outset of the nuclear industry, zirconium proved to be a good compromise between mechanical aspect and weak absorption properties in light water reactors.

### 14.2 Gurevich-Pomeranchuk Heterogeneous Resonant Absorption Theory

(Marchuk 1959, p. 167)

### 14.2.1 Theoretical Background

In 1943, Gurevich ${ }^{1}$ (1912-1992) and Pomeranchuk (1913-1966) ${ }^{2}$ proposed one of the first theories to allow for the heterogeneity effect of a thermal reactor on the absorption of a fuel cell using the effective absorption integral (direct

[^283]
measurements) in the framework of a Soviet uranium-graphite reactor program to produce plutonium for an atomic bomb [it was not until 1955 that this theory was published in (Atoms for peace 1955, volume V, pp. 528-534)]. From an educational and historical viewpoint [this theory is seldom described except in (Dresner 1960, p. 66)], some key elements of this model are recalled here. We consider a cell with fuel surrounded by a moderator where neutron scattering by heavy nuclides is ignored, to account only for scattering by light nuclides in the moderator. This hypothesis assumes a moderate fuel size compared to that of the moderator. Let us consider a fuel slab of thickness $d$ and surface area $S$ that has an incident neutron flux of $\Phi(E, x=0)$ perpendicularly. The fuel scattering cross section is composed of a resonant cross section $\Sigma_{x}^{R}$ and a potential cross section $\Sigma_{p}$. It is assumed ${ }^{3}$ that the fuel slab is thin enough for $\Sigma_{p} d \ll 1$. The neutron flux in the slab decays exponentially as:
$$
\Phi(E, x)=\Phi(E, 0) e^{-\Sigma_{t} x}
$$

The number of neutrons absorbed in the slab per unit energy can be calculated as:

$$
p(E)=S \Phi(E, 0) \int_{x=0}^{x=d} \Sigma_{a} e^{-\Sigma_{t} x} d x=S \Phi(E, 0) \frac{\Sigma_{a}}{\Sigma_{t}}\left(1-e^{-\Sigma_{t} d}\right)
$$

In the vicinity of the $j$ th resonance, the amount of neutrons absorbed by that resonance is obtained by integrating over the energy range "around" the resonance. For instance, by integrating over two resonance widths according to the BreitWigner model:

$$
\begin{aligned}
a_{j} & =\int_{E_{j}-\Gamma_{j}}^{E_{j}+\Gamma_{j}} p(E) d E \approx S \Phi\left(E_{j}, 0\right) \frac{\Sigma_{a}\left(E_{j}\right)}{\Sigma_{t}\left(E_{j}\right)} \int_{E_{j}-\Gamma_{j}}^{E_{j}+\Gamma_{j}}\left(1-e^{-\Sigma_{t} d}\right) d E \\
& =S \Gamma_{j} \Phi\left(E_{j}, 0\right) \frac{\Sigma_{a}\left(E_{j}\right)}{\Sigma_{t}\left(E_{j}\right)} \int_{0}^{+\infty}\left(1-e^{-\frac{\Sigma_{t}^{j}}{1+x^{2}} d}\right) d x
\end{aligned}
$$

It is assumed that the flux and the ratio of cross sections vary slowly in the range [ $E_{J}-\Gamma_{j}, E_{J}+\Gamma_{j}$ ], and a Breit-Wigner model for the total cross section is used (the integral is extended from 0 to infinity as per the justification given in the chapter on the Doppler effect). Finally, we obtain:

[^284]Absorption in a resonance for a slab geometry:

$$
\begin{equation*}
a_{j}=S d \Gamma_{j} \Phi\left(E_{j}, 0\right) \frac{\pi \Sigma_{a}\left(E_{j}\right)}{2} \frac{2}{\pi \Sigma_{t}\left(E_{j}\right) d} \int_{0}^{+\infty}\left(1-e^{-\frac{\Sigma_{t}^{j} d}{1+x^{2}}}\right) d x \tag{14.1}
\end{equation*}
$$

which is useful for the following function that can be calculated with Bessel functions:

$$
f(\beta)=\frac{2}{\pi \beta} \int_{0}^{+\infty}\left(1-e^{-\frac{\beta}{1+x^{2}}}\right) d x=e^{-\frac{\beta}{2}}\left(I_{0}\left(\frac{\beta}{2}\right)+I_{1}\left(\frac{\beta}{2}\right)\right)
$$

Analysis of this function shows that $f(\beta)=1+O(\beta)$ when $\beta \ll 1$ and that:

$$
f(\beta)=\frac{2}{\sqrt{\pi \beta}}\left(1+O\left(\frac{1}{\beta}\right)\right)
$$

when $\beta \gg 1$. At low values of $\beta$, the separation between resonances in this model is $\beta$ such that $\beta=\Sigma_{t}^{j} d \ll 1$ and for large values of $\beta$ such that $\beta=\Sigma_{t}^{j} d \gg 1$.

The previous approach can be extended to a fuel of any shape by assuming an isotropic flux $\Phi(\vec{r}, \vec{\Omega}, E)=\Phi(E, 0) /(4 \pi)$ that enables calculation of the number of incident neutrons on a surface area $d S$ of normal $\vec{n}$, i.e. $\vec{\Omega} . \vec{n} d S \Phi(E, 0) /(4 \pi)$. Similar reasoning leads to the calculation of the absorption per unit solid angle for a given resonance along a linear path $\ell$ through the fuel as:

$$
\begin{align*}
a_{j}(\vec{r}, \vec{\Omega}) & =\frac{\vec{\Omega} \cdot \vec{n} d S}{4 \pi} \Gamma_{j} \Phi\left(E_{j}, 0\right) \frac{\pi \ell \Sigma_{a}\left(E_{j}\right)}{2} \frac{2}{\pi \Sigma_{t}\left(E_{j}\right) \ell} \int_{0}^{+\infty}\left(1-e^{-\frac{\Sigma_{i}^{j} \ell}{1+x^{2}}}\right) d x  \tag{14.2}\\
& =\frac{\vec{\Omega} \cdot \vec{n} d S}{8} \Gamma_{j} \Phi\left(E_{j}, 0\right) \ell \Sigma_{a}\left(E_{j}\right) e^{-\frac{\Sigma_{t}^{j} \ell}{2}}\left(I_{0}\left(\frac{\Sigma_{t}^{j} \ell}{2}\right)+I_{1}\left(\frac{\Sigma_{t}^{j} \ell}{2}\right)\right)
\end{align*}
$$

The total absorption is obtained by integrating over the solid angles and over the external surface of the fuel:

$$
\begin{aligned}
a_{j} & =\int_{d S} \int_{\vec{\Omega}} p_{j}(\vec{r}, \vec{\Omega}) d \vec{\Omega} \\
& =V \frac{\pi \Gamma_{j}}{2} \Phi\left(E_{j}, 0\right) \Sigma_{a}\left(E_{j}\right) \frac{1}{4 \pi V} \int_{d S} d S \int_{\vec{\Omega}}|\vec{\Omega} \cdot \vec{n}| \ell e^{-\frac{\Sigma_{t}^{j}}{2}}\left(I_{0}\left(\frac{\Sigma_{t}^{j} \ell}{2}\right)+I_{1}\left(\frac{\Sigma_{t}^{j} \ell}{2}\right)\right) d \vec{\Omega}
\end{aligned}
$$

where $\ell$ depends only on the direction $\vec{\Omega}$ and on the volume, $V$ being the volume of the fuel:

$$
V=\frac{1}{4 \pi} \int_{d S} d S \int_{\vec{\Omega}}|\vec{\Omega} \cdot \vec{n}| \ell d \vec{\Omega}
$$

For a unit slowing-down density, the flux can be expressed as:

$$
\Phi\left(E_{j}, 0\right)=\frac{1}{\xi \Sigma_{s} E}
$$

In the previous equation, $\xi \Sigma_{s}$ corresponds to the complete cell (fuel + moderator). Since slowing down in the cell is due primarily to the moderator, we have:

$$
\xi \Sigma_{s} V_{\text {cell }} \approx \xi \Sigma_{s}^{M} V_{\text {Mod }}
$$

Equation (14.2) may be rewritten such that the previously-defined function $f\left(\beta \ell^{\prime}\right)$ is included and with the notations $\ell^{\prime}=d \ell$ where $d$ is the characteristic fuel thickness (Table 14.1):

$$
\left\{\begin{array}{l}
f\left(\beta \ell^{\prime}\right)=\frac{1}{4 \pi V} \int_{d S} d S \int_{\vec{\Omega}}|\vec{\Omega} \cdot \vec{n}| \ell e^{-\frac{\Sigma_{t}^{j} \ell^{\prime}}{2}}\left(I_{0}\left(\frac{\Sigma_{t}^{j} \ell^{\prime}}{2}\right)+I_{1}\left(\frac{\Sigma_{t}^{j} \ell^{\prime}}{2}\right)\right) d \vec{\Omega} \\
a_{j}=V \frac{\pi \Gamma_{j}}{2} \Phi\left(E_{j}, 0\right) \Sigma_{a}\left(E_{j}\right) f\left(\Sigma_{t}^{j} d\right)
\end{array}\right.
$$

Table 14.1 Relevant quantities for slab and cylindrical geometries

|  | $\|\vec{\Omega} \cdot \vec{n}\|$ | $\ell$ | $d \Omega$ | $f(\beta)$ |
| :--- | :--- | :--- | :--- | :--- |
| Slab geom- <br> etry <br> $\mu=\cos \theta$ | $\cos \theta$ | $\frac{1}{\cos \theta}$ | $\sin \theta d \theta$ | $f(\beta)=\int_{0}^{1} e^{-\frac{\beta}{2 \mu}}\left(I_{0}\left(\frac{\beta}{2 \mu}\right)+I_{1}\left(\frac{\beta}{2 \mu}\right)\right) d \mu$ |
| Cylindrical <br> geometry | $\sin \theta \cos \varphi$ | $\frac{\cos \varphi}{\sin \theta}$ | $\sin \theta d \theta d \varphi$ | $f(\beta)=\frac{4}{\pi} \int_{0}^{\frac{\pi}{2}} \cos ^{2} \varphi d \varphi \times$ |

The absorption summed over all the resonances is given by:

$$
A=\sum_{j} a_{j}=\sum_{\substack{j \text { such that } \Sigma_{t}^{j} d \ll 1 \\ j \text { such that } \Sigma_{t}^{j} d \gg 1}} V \frac{\pi \Gamma_{j}}{2} \Phi\left(E_{j}, 0\right) \Sigma_{a}\left(E_{j}\right) f\left(\Sigma_{t}^{j} d\right)
$$

In the case in which $\beta=\Sigma_{t}^{j} d \ll 1, f\left(\Sigma_{t}^{j} d\right) \approx 1$, while for the other case:

$$
f\left(\beta \ell^{\prime}\right)=\frac{2}{\sqrt{\pi \beta}}\left\langle\frac{1}{\sqrt{\ell^{\prime}}}\right\rangle\left(1+O\left(\frac{1}{\beta \ell^{\prime}}\right)\right)
$$

using the mean value for the inverse of the square root of the dimensionless chord:

$$
\left\langle\frac{1}{\sqrt{\ell^{\prime}}}\right\rangle=\frac{1}{4 \pi V} \int_{d S} d S \int_{\vec{\Omega}}|\vec{\Omega} \cdot \vec{n}| \ell \frac{1}{\sqrt{\ell^{\prime}}} d \vec{\Omega}
$$

Thus, the following quantity can be computed by substituting the Taylor expansions of $f$ in the equation for $a$ :

$$
\begin{aligned}
A= & \frac{V}{\xi \Sigma_{s}} \sum_{j \text { such that } \Sigma_{t}^{j} d \ll 1} \frac{\pi \Gamma_{j}}{2 E_{j}} \Sigma_{a}\left(E_{j}\right) \\
& +\left\langle\frac{1}{\sqrt{\ell}}\right\rangle \sum_{j \text { such that } \Sigma_{t}^{j} d \gg 1} \frac{\sqrt{\pi \Sigma_{t}\left(E_{j}\right) \Gamma_{j}^{2}}}{E_{j}} \frac{\Sigma_{a}\left(E_{j}\right)}{\Sigma_{t}\left(E_{j}\right)}
\end{aligned}
$$

usually expressed in terms of the effective resonance integral, through the resonance escape probability $p$ :

$$
A=1-p=\frac{N_{U} V}{\xi \Sigma_{s} V_{M o d}} I_{e f f}
$$

where $N_{U} V$ is the total number of absorbing atoms of uranium 238 in the cell volume.

### 14.2.2 Effective Resonance Integral

(Meghreblian and Holmes 1960, p. 640)
The effective resonance integral of uranium 238 can be written in the conventional form:

$$
I_{e f f}=a+\frac{b}{\sqrt{d}}
$$

By identification, the coefficients $a$ and $b$ in the expression can be determined by substituting the macroscopic cross sections by $N_{U} \sigma$ :

$$
\begin{aligned}
& a=\sum_{j \text { such that } \Sigma_{t}^{j} d \ll 1} \frac{\sigma_{a}\left(E_{j}\right)}{\sigma_{t}\left(E_{j}\right)} \frac{\pi \sigma_{t}\left(E_{j}\right) \Gamma_{j}}{2 E_{j}} b \\
&=\frac{1}{\sqrt{N_{U}}}\left\langle\frac{1}{\sqrt{\ell^{\prime}}}\right\rangle \sum_{j \text { such that } \Sigma_{i}^{j} d \gg 1} \frac{\sqrt{\pi \sigma_{t}\left(E_{j}\right) \Gamma_{j}^{2}}}{E_{j}} \\
& \frac{\sigma_{a}\left(E_{j}\right)}{\sigma_{t}\left(E_{j}\right)}
\end{aligned}
$$

In the 1950s, the resonances of uranium 238 were not well known, and coefficients $a$ and $b$ were evaluated experimentally. For cylindrical uranium metal rods, we have: $a_{c y l}=510^{-24} \mathrm{~cm}^{2}$ and $b_{c y l}=9.510^{-24} \mathrm{~cm}^{5 / 2}$, leading to determination of $I_{\text {eff }}$ in $\mathrm{cm}^{2}$ by taking $d$ in cm . For a non-cylindrical geometry:

$$
I_{e f f}=a_{c y l}+\frac{\left\langle\frac{1}{\sqrt{\ell}}\right\rangle^{\left\langle\frac{1}{\sqrt{\ell}}\right\rangle_{c y l}} \frac{b_{c y l}}{\sqrt{d}}}{\left\langle\frac{1}{}\right.}
$$

For a slab, the correction coefficient in front of $\frac{b_{c y l}}{\sqrt{d}}$ is equal to 0.685 .
This type of correlation for the effective resonance integral of uranium 238 has been developed in each country initiating a nuclear program in the 1950s under two generic forms:

$$
\begin{aligned}
& I_{\text {eff }{ }_{[b a r n]}}=A+B \frac{S}{M} \quad \text { or } \quad I_{\text {eff }[\text { barm }]} \\
& =C+D \sqrt{\frac{S}{M}} \text { depending on the individual country, }
\end{aligned}
$$

where $S / M$ is the fuel surface-to-volume ratio in $\mathrm{cm}^{2} / \mathrm{g}$ (Ligou 1982, p. 110). The coefficients $A$ and $B$ do not depend on the fuel geometry but vary with the fuel nature: oxide or metal (Heavy water lattices 1960, p. 81). Hence, for Magnox reactors, (Poulter 1963, p. 640) gives:

$$
I_{\text {eff } f_{\text {barn }]}}=5.65 \sqrt{1+\sum_{i \in \text { moderator }} \frac{N_{i} \sigma_{s, i}}{N_{U} \sigma_{s, U}}}+40.7 \frac{S_{\left[\mathrm{cm}^{2}\right]}}{M_{[\mathrm{g}]}}
$$

which is included in the resonance escape factor calculation:

$$
p=e^{--\frac{V_{U} N_{U} I_{\text {eff }}}{\sum_{i \in \text { moderator }} V_{i} N_{i}\left(\xi \quad \sigma_{S}\right)_{i}}}
$$

The Hellstrand formula (1962) for metallic uranium 238 at 293 K states that ${ }^{4}$ :

$$
I_{e f f}^{293 K}{ }_{[b a r n]}=2.81+24.7 \sqrt{\frac{S_{\left[c c^{2}\right]}}{M_{[g]}}}
$$

which is corrected with the fuel temperature effect (Doppler effect) by:

$$
I_{e f f}^{T}=I_{e f f}^{293 K}\left[1+0.01\left(0.51+0.5 \frac{S}{M}\right)\left(\sqrt{T_{[K]}}-\sqrt{293}\right)\right]
$$

### 14.3 Modeling the Pin Flux

The reactor core usually consists of hundreds, or even thousands, of elementary heterogeneous cells with fuel in a given form (rods, slabs, balls, etc.). The latter is surrounded by a cladding that prevents radioactive materials from disseminating in the nuclear facility, with a coolant. The role of the coolant is to transfer heat from the fuel towards the energy production system. For thermal neutron reactors, the coolant can itself be a moderator, as in the case of $P W R$, or the moderator can be separate, as in the case of $U N G G$ graphite-gas reactor. We will consider the flux calculation in an elementary heterogeneous cell.

[^285]
### 14.3.1 First-Collision Probability

The first-collision probability method was discussed in the chapter on the Boltzmann equation. The pin flux in a lattice is illustrated by the case of $P W R$ assemblies. The flux at a given position in a medium with patterns $j$ is given by:

$$
\Phi(\vec{r})=\sum_{j} \int_{V_{j}} q_{j}\left(\overrightarrow{r^{\prime}}\right) \frac{e^{-\overline{\Sigma_{t j} \ell}\left(\vec{r}, \vec{r}^{\prime}\right)}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}} d \overrightarrow{r^{\prime}}
$$

where $q_{j}\left(\overrightarrow{r^{\prime}}\right)=\Sigma_{s, j}\left(\overrightarrow{r^{\prime}}\right) \Phi_{j}\left(\overrightarrow{r^{\prime}}\right)+S_{j}\left(\overrightarrow{r^{\prime}}\right)$ is the source. The reaction rate in the volume $V_{i}$ is hence equal to the following, after integration over this volume:

$$
\int_{V_{i}} \Sigma_{t, i}(\vec{r}) \Phi(\vec{r}) d \vec{r}=\sum_{j} \int_{V_{i}} d \vec{r} \Sigma_{t, i}(\vec{r}) \int_{V_{j}} q_{j}\left(\overrightarrow{r^{\prime}}\right) \frac{e^{-\overline{\Sigma_{t j} \ell}\left(\vec{r}, \vec{r}^{\prime}\right)}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}} d \overrightarrow{r^{\prime}}
$$

Thus, the first-collision probability $\tilde{P}_{j, i}$ in volume $V_{i}$ produced by neutrons emitted isotropically by source $q_{j}$ in volume $V_{j}$ may be defined as follows:

$$
\tilde{P}_{j, i}=\frac{\int_{V_{i}} d \vec{r} \Sigma_{t, i}(\vec{r}) \int_{V_{j}} q_{j}\left(\overrightarrow{r^{\prime}}\right) \frac{e^{-\overline{\Sigma_{t j} \ell}\left(\vec{r}, \vec{r}^{\prime}\right)}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}} d \overrightarrow{r^{\prime}}}{\int_{V_{j}} q_{j}(\vec{r}) d \vec{r}}
$$

Under the hypothesis of homogeneous zones in which quantities are assumed to be constant in each zone, the following equation may be written:

$$
\int_{V_{j}} q_{j}(\vec{r}) d \vec{r}=\int_{V_{j}}\left(\Sigma_{s, j}(\vec{r}) \Phi_{j}(\vec{r})+S_{j}(\vec{r})\right) d \vec{r}=\left(\Sigma_{s, j} \Phi_{j}+S_{j}\right) V_{j}
$$

This is simply another method of defining mean flux:

$$
V_{j} \Phi_{j}=\int_{V_{j}} \Phi_{j}(\vec{r}) d \vec{r}
$$

and the average values:

$$
\begin{aligned}
& V_{j} \Sigma_{s, j} \Phi_{j}=\int_{V_{j}} \Sigma_{s, j}(\vec{r}) \Phi_{j}(\vec{r}) d \vec{r}, \\
& V_{j} S_{j}=\int_{V_{j}} S_{j}(\vec{r}) d \vec{r} \quad \text { and } \quad \int_{V_{i}} \Sigma_{t, i}(\vec{r}) \Phi(\vec{r}) d \vec{r}=V_{i} \Sigma_{t, i} \Phi_{i}
\end{aligned}
$$

Fig. 14.3 Zoning for a fuel pin


The discretized equation that relates the fluxes in several zones is:

$$
V_{i} \Sigma_{t, i} \Phi_{i}=\sum_{j} \tilde{P}_{j i} V_{j}\left(\Sigma_{s, j} \Phi_{j}+S_{j}\right)
$$

The probability $\tilde{P}_{j, i}$ includes a source term dependent on the flux, which is the quantity being sought. It may be assumed that zoning is fine enough for the sources to be uniform. In this case, the usual first-collision probabilities $P_{j, i}$ are obtained by simplifying by $q_{j}$, which has the same definition as $\tilde{P}_{j, i}$ except that the neutrons are emitted uniformly in volume $V_{j}$ :

First-collision probability in $i$ for a neutron emitted isotropically in $j$ :

$$
\begin{equation*}
P_{j, i}=\frac{\sum_{t, i} \int_{V_{i}} d \vec{r} \int_{V_{j}} \frac{e^{-\overline{t_{j} \ell}\left(\vec{r}, \vec{r}^{\prime}\right)}}{4 \pi\left|\vec{r}-\vec{r}^{\prime}\right|^{2}} d \overrightarrow{r^{\prime}}}{V_{j}} \tag{14.3}
\end{equation*}
$$

A set of zones is enclosed by a surface $S$, for instance the concentric zones of a fuel pin that are delimited by the outer surface of the pin. The probability of a neutron emitted in zone $i$ reaching surface $S$ is calculated as the complementary to one of the sum of probabilities of the neutron undergoing a collision in all the zones (Fig. 14.3):

$$
P_{i, S}=1-\sum_{j \in S} P_{i, j}
$$

The reciprocity theorem relates this probability to that for a neutron entering uniformly and isotropically through surface $S$ (current is proportional to $d S \vec{\Omega} . \vec{n}$ ) to undergo its first collision in zone $i$ :

$$
P_{S, i}=\frac{4 V_{i}}{S} P_{i, S} \Sigma_{t, i}
$$

The probability of a non-collided trajectory in the geometry being considered (the rod in the above example) is defined as:

$$
P_{S, S}=1-\sum_{j \in S} P_{S, j}
$$

### 14.3.2 The Amouyal-Benoist-Horowitz (A-B-H) Theory

(Barjon 1993, p. 579)
In 1956, this team that founded the neutron physics field in France proposed ${ }^{5}$ a new calculation method for thermal utilization factor $f$ (the probability of neutrons being absorbed in the fuel) of a $U N G G$ type cell, which forms the basis for methods currently used for heterogeneous reactor calculations. This approach accounts for the void channel (which contains carbon dioxide gas) in the $U N G G$ cell in an ingenious manner. The first pioneering work in the field dates back to Behrens $(1949)^{6}$ and Newmarch in 1955, who proposed that air channels be taken into account in British graphite-gas reactors ${ }^{7}$ using calculations in cylindrical geometry. The ABH method significantly improved the precision of these calculations. Similar work was carried out by Grant (1958) to allow for the streaming effect in gas channels, ${ }^{8}$ by generalizing Behrens' work through analytical corrections of the radial and longitudinal diffusion coefficients (Fig. 14.4).

### 14.3.2.1 Classical Thermal Utilization Factor Theory

The ratio of the mean flux in the moderator to that in the fuel is called the thermal (flux) disadvantage factor (Etherington 1957, pp. 6-77; Meghreblian and Holmes 1960, p. 645):

[^286]

Fig. 14.4 Report No 571 from ABH contains a diagram (often missing since it was printed on a separate sheet of paper) that reproduces on graph paper the extrapolation length $\lambda$ in terms of $c \Sigma_{m t}$, where $c$ is the inner radius of the graphite moderator and $\Sigma_{m t} \approx 0.3925 \mathrm{~cm}^{-1}$ the total cross section. The asymptotic value of 0.71 for the Milne problem is found here. The value of $\lambda$ is used in the calculation of the $1-f$ factor. (The Marguet collection)

$$
\zeta \equiv \frac{\Phi_{M}}{\Phi_{f}}
$$

The thermal utilization factor can be related to the thermal disadvantage factor using (Lamarsh and Baratta 2001, p. 313; Duderstadt and Hamilton 1976, p. 413):

$$
f=\frac{\Sigma_{a}^{c}}{\Sigma_{a}^{f}+\Sigma_{a}^{m} \frac{V_{m}}{V_{f}} \zeta}
$$

In a homogeneous reactor, the thermal utilization factor is readily calculated using the following formula (Littler and Raffle 1957, p. 113):

$$
\frac{1}{f}-1=\frac{\sum_{a}^{m}}{\Sigma_{a}^{f}} \equiv \frac{\text { absorption in the moderator }}{\text { absorption in the fuel }}
$$

If the medium is heterogeneous with two zones-fuel $f$ and graphite moderator $m$-by disregarding the gas channel and the cladding (Fig. 14.5 without graphite or cladding), this definition may be extended to the heterogeneous case:

Fig. 14.5 Neutron density in the $U N G G$ cell [from (Littler and Raffle 1957, p. 105)]


$$
\begin{aligned}
\frac{1}{f} & -1=\frac{V_{m} \Sigma_{a}^{m} \overline{\Phi_{m}}}{V_{c} \Sigma_{a}^{c} \overline{\Phi_{c}}} \equiv \frac{\text { absorption in the moderator }}{\text { absorption in the fuel }} \\
& \equiv \frac{V_{m} \Sigma_{a}^{m}}{V_{f} \Sigma_{a}^{c}} \underbrace{\frac{\Phi(a)}{\overline{\Phi_{f}}}}_{G}+\underbrace{\frac{V_{m} \Sigma_{a}^{m}}{V_{f} \Sigma_{a}^{c}} \frac{\overline{\Phi_{m}}-\Phi(a)}{\overline{\Phi_{f}}}}_{x}
\end{aligned}
$$

The coefficient $G$ reflects the fact that the flux decreases in the fuel and $X$ is an excess of captures dependent solely on the flux spectrum in the moderator, using the notations of Guggenheim and Pryce. ${ }^{9}$ These two coefficients can be calculated in the classical theory of thermal scattering in a cylindrical medium where the thermal neutron source originates from the graphite moderator:

$$
\left\{\begin{array} { l } 
{ \Delta \Phi _ { c } - \frac { \Sigma _ { a , c } } { D _ { c } } \Phi _ { c } = 0 } \\
{ \Delta \Phi _ { m } - \frac { \sum _ { a , m } } { D _ { m } } \Phi _ { m } = - \frac { q } { D _ { m } } }
\end{array} \text { with: } \left\{\begin{array} { l } 
{ \kappa _ { c } ^ { 2 } \equiv \frac { \Sigma _ { a , c } } { D _ { c } } } \\
{ \kappa _ { m } ^ { 2 } \equiv \frac { \Sigma _ { a , m } } { D _ { m } } }
\end{array} \text { and } \left\{\begin{array}{l}
\Phi_{c}(a)=\Phi_{m}(a) \\
-\left.D_{m} \frac{\partial \Phi_{m}}{\partial r}\right|_{a}=-\left.D_{c} \frac{\partial \Phi_{c}}{\partial r}\right|_{a} \\
-\left.D_{m} \frac{\partial \Phi_{m}}{\partial r}\right|_{b}=0 \text { and }-\left.D_{c} \frac{\partial \Phi_{c}}{\partial r}\right|_{0}=0
\end{array}\right.\right.\right.
$$

With all calculations done, we obtain:

$$
\left\{\begin{array}{l}
G=\frac{\kappa_{c} a I_{0}\left(\kappa_{c} a\right)}{2} \frac{I_{1}\left(\kappa_{c} a\right)}{I_{1}} \\
X=\frac{\kappa_{m}\left(b^{2}-a^{2}\right)}{2 a} \frac{K_{0}\left(\kappa_{m} a\right)+\frac{K_{1}\left(\kappa_{m} b\right)}{I_{1}\left(\kappa_{m} b\right)} I_{0}\left(\kappa_{m} a\right)}{K_{1}\left(\kappa_{m} a\right)+\frac{K_{1}\left(\kappa_{m} b\right)}{I_{1}\left(\kappa_{m} b\right)} I_{1}\left(\kappa_{m} a\right)}-1
\end{array}\right.
$$

[^287]
### 14.3.2.2 A-B-H Theory for the Thermal Utilization Factor ${ }^{10}$

The principle consists in representing a channel in a $U N G G$ reactor as a fuel pin of volume $V_{f}$ surrounded by a "void" channel of carbon dioxide gas (neutron collisions

[^288]in that channel are ignored), itself surrounded by a graphite moderator of volume $V_{m}$. The innovative idea was to use methods incorporating elements of neutron transport (collision probabilities) and of diffusion. Assuming that neutrons are not slowed down to thermal energy in the fuel, slowing down on light nuclides (oxygen) in the fuel can be disregarded. Thus, it is assumed that the graphite moderator is a uniform source of thermal neutrons and that this source is zero in the fuel. Furthermore, capture reactions in the moderator are not considered. Thermal neutron distribution is calculated using elementary diffusion theory with a rise in uniform flux at the graphite surface. This rise does not depend on the cell
the studies to be executed. They were the only ones with the know-how, and thus were the only ones to have access to this equipment. Hence, they were organized into several application sub-groups with one of sub-groups being dedicated to the base programs delivered by the manufacturers, to designing basic sub-programs, and to operating the machines. The application sub-groups were required to design programs to solve problems submitted by the engineers and physicists with the Department on one hand, and more straightforward problems of general value on the other.

The majority of requests came from the neutron physicists in the department, while the othersvery few-emanated from the theoretical physics department. The IBM 650, which had a relatively limited capacity, was very useful and was successfully utilized for numerous problems that were too complex for the calculation team. For instance, there were cases of neutron physics problems in diffusion theory with one space variable, but with a nearly infinite number of media, and two neutron groups: this progress was greatly appreciated. MERCURY, was far more powerful than the IBM 650, and opened up new possibilities with the solution of problems involving two spatial variables. However, because of its fragile nature, calculations were restricted to under two hours, otherwise the poor technical inspector responsible for maintenance was in a panic since the probability of unpredictable stoppage of the machine was no longer negligible, and this could lead to appreciable worsening of the monthly breakdown rate, resulting in penalties for the constructor. The operation of the machine was very "low-tech" and simple. Indeed, the working day was essentially dedicated to tests, and each engineer executed his calculations himself on the computer, directly at the workstation of the IBM 650 or the MERCURY. The duration of these calculations was highly unpredictable, as the schedules could only be very approximate. Time loss could not be avoided and affected the cost-effectiveness of the machines, but it was difficult to proceed otherwise as calculations could not be batch-processed at the time. Since it was impossible to answer all the programming requests from all the departments within a reasonable time, the specialized team from the Mathematical Physics Department set up an introductory programming course for all those interested. The latter was simplified on MERCURY thanks to a simple language (the "Autocode"), which was very successful. This led to an increase in the number of users, hence in the number of requirements for calculations. This situation resulted in saturation of the MERCURY machine, but in 1959, the Department of Military Applications bought a new machine, an IBM 704, with 30\% of its time being given over to the civil sector of the CEA. This allowed for more time in the acquisition of a new machine. The study of this new project began in 1959, and two choices quickly emerged: a GAMMA 60 from the Bull Company, and an IBM 7090. The GAMMA 60 had very innovative features but was not yet ready for use. It was reminiscent of the situation of the MERCURY machine bought previously, and an IBM 7090 was ordered in 1960 and installed in 1961 in a new building, constructed especially for the occasion, at Saclay."

Extract from "Deuxième Colloque sur l'Histoire de l'Informatique en France" (Second conference on the history of computing in France), Papers edited by Philippe Chatelin and Pierre-E. Mounier-Kuhn, Conservatoire National des Arts et Métiers, Paris, March 1990; 2 vol. (366+368 pages +21 p. additional) ISBN 2-9502887-3-1, pp. 11-28.
shape, and takes into account the anisotropy around the fuel pin. Since the migration area of neutrons in graphite is much larger than the pitch between the channels, these previous hypotheses remain acceptable. Finally, it is also assumed that the cell is in an infinite lattice (with no neutron current between the cells), a hypothesis employed for any lattice calculation. The following notations, adapted from a presentation of P. Benoist's work, ${ }^{11}$ are used (Photo 14.1):
$P_{i, j}$ is the probability of a neutron emitted uniformly and isotropically in medium $I$ undergoing its first collision in medium $j$.
$P_{i, j}^{*}$ is the probability of a neutron emitted uniformly and isotropically in medium $i$ being absorbed in medium $j$.
$P_{i, i}^{+}$is the probability of a neutron emitted uniformly and isotropically in medium $i$ being absorbed in medium $i$ without leaving the cell (self-absorption).

Let $S$ be a convex surface surrounding the fuel pin (for example, the surface of the rod itself, Fig. 14.6):
$P_{f, S}^{+}=1-P_{f, f}^{+}$is the probability for a neutron emitted uniformly and isotropically
in the fuel medium reaching surface $S$ and exiting the fuel. This is the same as the
multi-collision leakage probability denoted as $P_{V S}$ in the chapter on the
Boltzmann equation.
$P_{S, f}^{+}$is the probability of a neutron emitted uniformly and isotropically on surface
$S$ being absorbed in the fuel medium without crossing $S$ again.
$P_{S, f}^{*}$ is the probability of a neutron emitted uniformly and isotropically on surface
$S$ being absorbed in the fuel medium, possibly by crossing $S$ again.

By definition, the thermal utilization factor which represents the probability of a neutron being efficient, i.e of it being absorbed in the fuel, is written as:

$$
f=P_{m, f}^{*}
$$

within the hypothesis that the sources located in the moderator are isotropic and uniform in one energy group theory (fast neutrons are emitted in the fuel and are slowed down to create a thermal slowing-down source in graphite), and assuming that there is no leakage thanks to reflective boundary conditions with modeling of an infinite lattice.

[^289]

Photo 14.1 CEA Report No. 571 by A. Amouyal and P. Benoist, under the supervision of J. Horowitz, is often cited in several reference works. Published in 1956 with 34 typewritten pages, it is considered a forerunner of the heterogeneous collision probability method, $P_{i, j}$. (The Marguet collection)

The approach of Amouyal, Benoist and Horowitz (ABH model) involves considering the absorption of monokinetic neutrons in the fuel as a negative source (this approach was previously discussed in the Galanin model) and computing the outgoing probability for these hypothetical neutrons in transport theory.

$$
f=P_{m, f}^{*}=\frac{\Sigma_{a}^{f}}{V_{m}} \int_{V_{m}} d V_{m} \int_{V_{f}} d V_{f} G\left(\overrightarrow{r_{m}} \rightarrow \overrightarrow{r_{f}}\right)
$$

where $G\left(\overrightarrow{r_{m}} \rightarrow \overrightarrow{r_{f}}\right)$ is the Green function of the transport operator, i.e. the flux at a given position in the fuel due to a unit source placed in the moderator at $\overrightarrow{r_{m}}$. In monokinetic theory only, the reciprocity theorem can be used such that:


Fig. 14.6 $U N G G$ channel

$$
G\left(\overrightarrow{r_{m}} \rightarrow \overrightarrow{r_{f}}\right)=G\left(\overrightarrow{r_{f}} \rightarrow \overrightarrow{r_{m}}\right)
$$

Hence, $P_{f, m}^{*}$ is introduced in the equation as:

$$
f=\frac{\Sigma_{a}^{f}}{V_{m}} \frac{V_{f}}{\Sigma_{a}^{m}} \frac{\Sigma_{a}^{m}}{V_{f}} \int_{V_{m}} d V_{m} \int_{V_{f}} d V_{f} G\left(\overrightarrow{r_{f}} \rightarrow \overrightarrow{r_{m}}\right)=\frac{\Sigma_{a}^{f}}{V_{m}} \frac{V_{f}}{\Sigma_{a}^{m}} P_{f, m}^{*}
$$

It may be seen that $P_{f, m}^{*} \approx P_{f, S}^{+} P_{S, m}^{*}$, i.e. the product of the leakage probability and the conditional probability $P_{S, m}^{*}$ of a neutron leaking from the fuel being absorbed in the moderator. Strict equality does not occur since outgoing neutrons from surface $S$ are not systematically isotropic. Thus, it could be written that $P_{f, m}^{*}$ $=P_{f, S}^{+} P_{S, m}^{\#}$ where $P_{S, m}^{\#}$ is the probability of a neutron emitted non-uniformly from $S$ being absorbed in the moderator. In a sense, $P_{S, m}^{\#} \approx 1-f$. In fact, $P_{S, m}^{\#}<1-f$ since a neutron entering the moderator from surface $S$ has less chance of being absorbed than a neutron emitted by a uniform source in the moderator.
where:

$$
f=\frac{\Sigma_{a}^{f}}{V_{m}} \frac{V_{f}}{\Sigma_{a}^{m}} P_{f, S}^{+} P_{S, m}^{\#}=\frac{\Sigma_{a}^{f}}{V_{m}} \frac{V_{f}}{\Sigma_{a}^{m}} P_{f, S}^{+}\left[(1-f)-\left(1-f-P_{S, m}^{\#}\right)\right]
$$

that is:
Amouyal-Benoist-Horowitz formula:

$$
\begin{equation*}
\frac{1}{f}-1=\frac{V_{m} \Sigma_{a}^{m}}{V_{f} \Sigma_{a}^{f} P_{f, S}^{+}}+\frac{1-f-P_{S, m}^{\#}}{f} \tag{14.4}
\end{equation*}
$$

Assuming $P_{S, m}^{\#} \approx 1-f$, an approximation for $(1-f) / f$ is obtained:

$$
\frac{1}{f}-1 \approx \frac{V_{m} \Sigma_{a}^{m}}{V_{f} \Sigma_{a}^{f} P_{f, S}^{+}}
$$

This approximation can be improved by assuming that $P_{S, m}^{\#}=P_{S, m}^{*}$ and calculating:

$$
P_{S, m}^{*}=P_{S, m}^{+}+\left(1-P_{S, m}^{+}\right) P_{f S S m}
$$

which means that the probability of an outgoing neutron exiting the fuel through $S$ being captured in the moderator is equal to the probability of direct capture without passing through $S$, added to the probability of passing through $S$ again before being captured. A new capture probability $P_{f S S m}$ is defined for a neutron emitted from the fuel and having crossed $S$ at least twice. Following the same reasoning (Fig. 14.7):

$$
1-f=P_{m, m}^{*}=P_{m, m}^{+}+\left(1-P_{m, m}^{+}\right) P_{m S m} \text { or even: } f=\left(1-P_{m, m}^{+}\right)\left(1-P_{m S m}\right)
$$

where $P_{m S m}$ is the capture probability in the moderator for a neutron emitted in the moderator and having crossed $S$ for the first time. The probabilities $P_{f S S m}$ and $P_{m S m}$ differ only in terms of the angular distribution of the neutrons being considered and are thus very close.

Fig. 14.7 Definition of probabilities in $A-B-H$


$$
\begin{aligned}
\frac{1-f-P_{S m}^{\#}}{f} & =\frac{P_{m, m}^{+}+\left(1-P_{m, m}^{+}\right) P_{m S m}-P_{S, m}^{+}-\left(1-P_{S, m}^{+}\right) P_{f S S m}}{\left(1-P_{m, m}^{+}\right)\left(1-P_{m S m}\right)} \\
& =\frac{\left(1-P_{S, m}^{+}\right)\left(1-P_{f S S m}\right)-\left(1-P_{m, m}^{+}\right)\left(1-P_{m S m}\right)}{\left(1-P_{m, m}^{+}\right)\left(1-P_{m S m}\right)}
\end{aligned}
$$

Assuming that these neutrons all originate from the moderator, it may be considered that isotropic scattering after several collisions has "erased" the history and that $P_{f S S m}=P_{m S m}$. Even if the angular distribution of neutrons leaving the fuel is highly anisotropic, the impact on capture in the moderator is insignificant. It can also be seen that even though capture in the rod depends strongly on the angular distribution of incoming neutrons, the probability $P_{S, c}^{+}$can be justifiably employed. Thus:

$$
\frac{1-f-P_{S m}^{\#}}{f}=\frac{P_{m, m}^{+}-P_{S, m}^{+}}{1-P_{m, m}^{+}}=\frac{1-P_{m, S}^{+}-P_{S, m}^{+}}{P_{m, S}^{+}}
$$

Probabilities $P_{m, S}^{+}$and $P_{S, m}^{+}$can be related. Let us consider a moderating medium that fills up the whole space and in which thermal neutron sources are constant. The flux of this theoretical case is flat and isotropic. If in this medium, a zone of volume $V_{m}$ surrounded by a surface $S$, is delimited, the absorption rate integrated in this volume is equal to that induced by neutrons not exiting through the surface, and by those entering through the surface on which the angular current is equal to $\Phi / 4$, as we saw in the section on diffusion theory:

$$
V_{m} \Sigma_{a}^{m} \Phi=\underbrace{V_{m} \Sigma_{a}^{m} \Phi P_{m, m}^{+}}_{\text {in the volume }}+\underbrace{S \frac{\Phi}{4} P_{S, m}^{+}}_{\text {from the surface }}
$$

Thus:

$$
P_{S, m}^{+}=\frac{4 V_{m}}{S} \sum_{a}^{m}\left(1-P_{m, m}^{+}\right)=\frac{4 V_{m}}{S} \sum_{a}^{m} P_{m, S}^{+}
$$

With the same reasoning: $P_{S, f}^{+}=\frac{4 V_{f}}{S} \Sigma_{a}^{f} P_{f, S}^{+}$. Hence, the corrective factor in the $A-B-H$ formula is equivalent to a fuel-outgoing probability $P_{f, S}^{+}$calculation after any number of collisions. If the flux is uniform (i.e. the neutrons scattered in the fuel have uniform distribution):

$$
P_{f, S}^{+}=\underbrace{P_{f, S}}_{\text {first collision }}+\underbrace{\frac{\Sigma_{s, f}}{\Sigma_{t, f}} P_{f, f} P_{f, S}^{+}}_{\text {scattered neutrons }}
$$

Thus:

$$
P_{f, S}^{+}=\frac{1-P_{f, f}}{1-\frac{\Sigma_{s, f}}{\Sigma_{t, f}} P_{f, f}}
$$

The probability $P_{f, f}$ is calculated analytically for a fuel pin of radius $R$ by integration of Bessel functions:

$$
P_{f, f}(R)=1-2 R \Sigma_{t, f} \int_{x=R \Sigma_{t, f}}^{+\infty} \frac{I_{1}(x) K_{1}(x)}{x^{2}} d x
$$

The calculation of $f$ leads to the thermal disadvantage factor:

$$
\zeta=\frac{\Sigma_{a}^{f} V_{f}}{\Sigma_{a}^{m} V_{m}}\left(\frac{1}{f}-1\right)
$$

The $A-B-H$ method significantly improved the precision of calculations for the first French $U N G G$. It is famous at the international level as a landmark of the multicell approach (Duderstadt and Hamilton 1976, p. 414; Stacey 2001, p. 515). From 1957 onwards, B. Bailly du Bois considerably developed ${ }^{12}$ the analytical calculation of the radial moderator flux in cells for several geometries in infinite twiceperiodic lattices, through advanced use of pole theory (residue theorem) ${ }^{13}$ to obtain non-singular solutions for the diffusion equation in the moderator. These calculations correct the thermal utilization factor $f$ and the resonance escape probability factor $p$ (using a Fermi age slowing-down model) by taking into account the cell geometry. It is shown that $f$ is weakly sensitive to the flux distribution in the moderator. Pierre Benoist subsequently proposed ${ }^{14}$ an advanced theory for the diffusion coefficient in a lattice with cavities (similar to $U N G G$ ). This takes into account the first-collision probabilities using a heterogeneous multi-cell approach, leading to calculation of the ratio of mean diffusion coefficient in the cell to the moderator coefficient.

[^290]

Pierre J. Benoist is among the most notable French theoretical physicists in the field of neutron physics (Courtesy Benoist)


### 14.3.3 Multi-cell Approach in Two Dimensions

### 14.3.3.1 Context

The goal is to extend the approach to a lattice of identical pins that will be assumed as being infinite for the time being (Fig. 14.8).

In order to calculate all collision probabilities $P_{i, j}$ in each zone of the lattice, the problem can be simplified by using the regularity of the lattice. Since calculations are simpler in one dimension, the cells can be approximated by a cylindrical geometry. This is a non-trivial operation and requires discussion (Fig. 14.9):

The cylindrical approximation for a rectangle can be carried in several ways. Either the amount of matter or the outer surface of the cell can be retained. The surface to conserve is equal to $a b$, and the perimeter is $2(a+b)$.

Historically, Wigner-Seitz ${ }^{15}$ proposed the conservation of the surface, thus retaining the amount of matter (Stamm'ler and Abbate 1983, p. 40), while J.R. Askew suggested retaining the outer perimeter so as to preserve the leakage term. ${ }^{16}$ To conserve the amount of matter in the Askew model, the density of the cell must be decreased. J. C. Lefebvre proposed an intermediate approach that leads to the Wigner formulae in the case of a square cell while being more realistic on the perimeter for the rectangular cell (this situation exists even in $P W R$ if the water gap between assemblies is modeled) (Table 14.2).

[^291]

[^292]

Fig. 14.8 Regular lattice of cells $(P W R$ case $)$


Fig. 14.9 Cylindrical approximation for a rectangle

Table 14.2 Cylindrical approximations

| Cylindrical approximations for a rectangle $(a \times b)$ | Wigner-Seitz | Askew | Lefebvre |
| :--- | :--- | :--- | :--- |
| Equivalent area | $a b$ | $\frac{(a+b)^{2}}{\pi}$ | $\frac{(a+b)^{2}}{4}$ |
| Density | $\rho$ | $\rho \frac{\pi a b}{(a+b)^{2}}$ | $\rho \frac{4 a b}{(a+b)^{2}}$ |
| Equivalent perimeter | $2 \sqrt{\pi a b}$ | $2(a+b)$ | $(a+b) \sqrt{\pi}$ |
| Equivalent radius | $\sqrt{\frac{a+b}{\pi}}$ | $\frac{a+b}{\pi}$ | $\frac{a+b}{\sqrt{2 \pi}}$ |

The Roth formalism consists in taking the cylindrical approximation for a fuel cell and recommends substitution of the specular reflective conditions (mirror reflection-Descartes' reflection laws) by an isotropic reflection condition (Fig. 14.10), also called white reflection. Studies ${ }^{17}$ have nevertheless shown that this method tends to underestimate the $k_{\infty}$ with respect to a Monte Carlo calculation in exact geometry ( $0.2 \%$ for a $U O X$ fuel and up to $0.5 \%$ for a MOX pin). Thus, the heterogeneity effect proves to be more significant in a square cell where the outer surface is not at a constant distance from the fuel as is the case for the cylindrical

[^293]Specular reflection


O Isotropic reflection


Fig. 14.10 Specular and isotropic reflections
cell. Further, he assumed that the outgoing currents are uniform, which is equivalent to the fact that an incoming neutron with a direction $\vec{\Omega}$ has an equal probability of exiting without any collisions in the two-dimensional cell with any direction $\overrightarrow{\Omega^{\prime}}$. This reasoning is not correct for the backwards direction $-\vec{\Omega}$ given that no collision could force the neutron backwards. Thus, the probability of return via the true side through which the neutron entered is biased in this approach. The uniform current approximation should also be employed cautiously in a heterogeneous cell. For an incoming neutron, the solid angle in which the neutron may cross the fuel tends to decrease the probability of the neutron exiting by the opposite side (shadowing effect of the fuel pin). This effect depends on the energy of the incident neutron since neutrons whose energy coincides with that of the resonances of isotopes in the pin will be preferentially absorbed.

### 14.3.3.2 Dancoff-Ginsburg Factor



A very rare photograph of Sydney Dancoff, here with his baby daughter, Anita (The Marguet collection, Photograph unknown)

In a heterogeneous lattice constituted of fuel surrounded by moderator, there is a shadowing effect due to the fact that some neutrons cannot reach the fuel pin since it is absorbed in surrounding pins. This effect is particularly important for closed-pack lattices, and modifies the absorption integral by a corrective term set up by Dancoff ${ }^{18}$ and Ginsburg. ${ }^{19}$ Let $P_{i, j}^{+}$be the probability, dubbed intern, that a neutron emitted uniformly and isotropically in a volume $V_{i}$ interacts in volume $V_{j}$ without leaving the cell by surface $S$. These probabilities can be calculated by noting that the probability $P_{i, j}$ is equivalent to an infinite sum of probabilities of the type $P_{i, j}^{+}$for the adjacent cells crossed:


Since all the cells are identical, the probability of travelling through a cell without collision $P_{S, S}^{+}$is the same for all cells. This value is naturally smaller than 1 , and thus:

[^294]Dancoff formula:

$$
\begin{equation*}
P_{i, j}=P_{i, j}^{+}+\frac{P_{i, S}^{+} P_{S, j}^{+}}{1-P_{S, S}^{+}} \tag{14.5}
\end{equation*}
$$

The corrective coefficient $P_{i, S}^{+} P_{S, j}^{+} /\left(1-P_{S, S}^{+}\right)$is called the Dancoff-Ginsburg factor, often denoted $C$ (Duderstadt and Hamilton 1976, p. 434; Stamm'ler and Abbate 1983, p. 296; Ferziger and Zweifel 1966, p. 121; Silvennoinen 1976, p. 150). In 1944, these authors established the coefficient to characterize the probability of a neutron emitted from the fuel reaching the surface of another fuel pin in another cell without collision (Stamm'ler and Abbate 1983, p. 296). It integrates the fact that a neutron can travel directly from one zone $i$ of a cell to another zone $j$ by leaving the cell in a multi-cell approach, e.g. a neutron that goes from a pin to another pin without any collision in water. In the case of a geometry with a fuel pin surrounded by water, the following are denoted: $f$ for the fuel, $S$ is the fuel surface and $F$ the outer boundary of the cell. In this case, the Dancoff-Ginsburg factor $C$, which is the average probability of reaching the surface of another fuel pin without collision (regardless of its distance, it is an average value: in water reactors, $C$ is approximately 0.2 ), must be distinguished from the probability $P_{S, S}^{+}$, which is that of a neutron entering the fuel and travelling through it (Fig. 14.11).


Fig. 14.11 Dancoff-Ginsburg problem


By noticing that in this geometry, $P_{f, S}^{+}=1-P_{f, f}^{+}$, and with the reciprocity theorem:

$$
P_{S, f}^{+}=\frac{4 V_{f}}{S} \Sigma_{t, f} P_{f, S}^{+}=\frac{4 V_{f}}{S} \Sigma_{t, f}\left(1-P_{f, f}^{+}\right)
$$

Hence, we obtain an explicit calculation of $P_{c, c}$ in terms of $P_{c, c}^{+}$and $P_{S, S}^{+}$. It should be noted that the "return" effect must be accounted for cautiously, i.e. the probability of a neutron leaving the cell and returning without collision in the fuel is counted in the Dancoff-Ginsburg factor. Similarly, the successive paths through the various cells without collision in the other cells are counted. $C$ can be expressed from outgoing probabilities of the cell with surface $F$ :

$$
C=P_{f, F}^{+} P_{F, f}^{+}+P_{f, F}^{+} P_{F, F}^{+} P_{F, f}^{+}+P_{f, F}^{+}\left(P_{F, F}^{+}\right)^{2} P_{F, c}^{+}+\cdots=\frac{P_{f, F}^{+} P_{F, f}^{+}}{1-P_{F, F}^{+}}
$$

The works of Rothenstein (in 1959) and later Fukai (in 1960) ${ }^{20}$ led to analytical calculation of the Dancoff coefficient for geometries with cylindrical rods. The recent work of A . Talamo should also be highlighted for the analytical calculation for high-temperature prismatic reactors. ${ }^{21}$

[^295]
### 14.3.3.3 The Dancoff Effect in Different Geometries: Shielding Problems

Let us consider a fuel cylinder placed vertically in a moderator of total cross section $\Sigma_{t}$. The fuel contains a resonant isotope that absorbs all neutrons having an energy close to that of a resonance. Thus, it is a perfect shield for that particular energy value. But scattering in the moderator can be considered as a source of thermal neutrons.

The neutron current emitted in the volume element $d V$ with unit volume neutron source $q$ and belonging to the cylinder (pin) represented in Fig. 14.12 across the surface $d S$ is given by:

$$
d J=q d V \cos \theta \frac{r}{R} \frac{e^{-\Sigma_{l} R}}{4 \pi R^{2}}
$$

The coefficient $\cos \theta \frac{r}{R}$ corresponds to the non-shadowed factor since $r$ is the projection of the distance $R$ between the source and the element $d S$ in the plane $O x y$. Assuming that the pin is infinite along the $z$ axis, after integration, the following equation is obtained:

$$
J(\theta)=\int_{z=-\infty}^{z=+\infty} d J=q d A r \cos \theta \int_{z=-\infty}^{z=+\infty} \frac{e^{-\Sigma_{l} R}}{4 \pi R^{3}} d z
$$

It should be pointed out that $R^{2}=r^{2}+z^{2}$, thus $2 R d R=2 z d z$ as long as $r$ is constant while $z$ varies. Using the change of variable:

$$
\operatorname{ch} \tau=R / r \quad \text { and } \quad s h \tau=\sqrt{c h^{2} \tau-1}=\sqrt{\left(R^{2}-r^{2}\right) / r^{2}}=z / r
$$

the equation is transformed as:


Fig. 14.12 Cylindrical geometry

$$
J(\theta)=q d A \quad r \cos \theta \int_{\tau=-\infty}^{\tau=+\infty} \frac{e^{-\Sigma_{l} r c h \tau}}{4 \pi r^{3} c h^{3} \tau} r c h \tau d \tau=q \frac{d A \cos \theta}{4 \pi r} \int_{\tau=-\infty}^{\tau=+\infty} \frac{e^{-\Sigma_{l} r c h \tau}}{c h^{2} \tau} d \tau
$$

This is a Bickley-Nayler function which has the following major properties:

$$
\begin{aligned}
& K I_{n}(x) \equiv \int_{\tau=0}^{\tau=+\infty} \frac{e^{-x c h \tau}}{c h^{n} \tau} d \tau=\frac{1}{(n-1)!} \int_{\tau=x}^{\tau=+\infty}(t-x)^{n-1} K I_{0}(\tau) d \tau \\
& =\frac{x^{n}}{(n-1)!} \int_{\tau=1}^{\tau=+\infty}(t-1)^{n-1} K I_{0}(x \tau) d \tau=\int_{\tau=1}^{\tau=+\infty} \frac{e^{-x \tau}}{t^{n} \sqrt{t^{2-1}}} d \tau \\
& K I_{n}(x) \equiv \int_{\theta=0}^{\theta=\frac{\pi}{2}} \cos ^{n-1}(\theta) e^{-\frac{x}{\cos \theta}} d \theta=\int_{\theta=0}^{\theta=\frac{\pi}{2}} \sin ^{n-1}(\theta) e^{-\frac{x}{\sin \theta}} d \theta
\end{aligned}
$$

Further, $K I_{0}(x)=K_{0}(x)$, the modified Bessel function (thus the term $K I$ for the Bickley-Nayler function):

$$
K I_{2 n}(0)=\frac{\Gamma(n) \Gamma\left(\frac{3}{2}\right)}{\Gamma\left(n+\frac{1}{2}\right)}, \quad K I_{2 n+1}(0)=\frac{\frac{\pi}{2} \Gamma\left(n+\frac{1}{2}\right)}{\Gamma\left(\frac{1}{2}\right) \Gamma\left(n+\frac{1}{2}\right)}
$$

The Bickley-Nayler functions obey the following recurrence formula:

$$
n K I_{n+1}(x)=(n-1) K I_{n-1}(x)-x K I_{n}(x)+x K I_{n-2}(x) \quad n \geq 2
$$

The most precise asymptotic expansion has been obtained by Zekeriya Altaç:
$K I_{n}(x) \approx \sqrt{\frac{\pi}{2 x}} e^{-x}\left[\begin{array}{l}1-\frac{(m+1)}{X}+\frac{3\left(m^{2}+6 m+3\right)}{2!X^{2}}-\frac{15(m+5)\left(m^{2}+10 m+3\right)}{3!X^{3}} \\ +\frac{105\left(m^{4}+28 m^{3}+242 m^{2}+644 m+105\right)}{4!X^{4}} \\ -\frac{945(m+9)\left(m^{4}+36 m^{3}+386 m^{2}+1116 m+105\right)}{5!X^{5}} \\ +\frac{10395\left(m^{6}+66 m^{5}+1645 m^{4}+19140 m^{3}+102439 m^{2}+198594 m+10395\right)}{6!X^{6}}\end{array}\right]$
$\times$ with $m \equiv 4 n$ and $X \equiv 8 x$
From the previous properties:

$$
\int_{\tau=-\infty}^{\tau=+\infty} \frac{e^{-\Sigma_{t} r c h \tau}}{c h^{2} \tau} d \tau=2 \int_{\tau=0}^{\tau=+\infty} \frac{e^{-\Sigma_{t} r c h \tau}}{c h^{2} \tau} d \tau \equiv 2 K I_{2}\left(\Sigma_{t} r\right)
$$

i.e. for the calculation of $J(\theta)$ :

$$
J(\theta)=q \frac{d A \cos \theta}{2 \pi r} K I_{2}\left(\Sigma_{t} r\right)
$$

This equation is valid for any surface element $d A$. The current emitted by a cylinder with any type of cross section is expressed as:

$$
J=\frac{q}{2 \pi} \int_{A} d A \frac{\cos \theta}{r} K I_{2}\left(\Sigma_{t} r\right)
$$

A particular case is that in which the fuel fills up the half-space delimited by $x>0$. Since $\frac{d K I_{n}(x)}{d x}=-K I_{n-1}(x)$ :
$J=\frac{q}{2 \pi} \int_{\theta=-\frac{\pi}{2}}^{\theta=+\frac{\pi}{2}} \int_{r=0}^{r=+\infty} r d r d \theta \frac{\cos \theta}{r} K I_{2}\left(\Sigma_{t} r\right)=\frac{q}{\pi} \int_{r=0}^{r=+\infty} K I_{2}\left(\Sigma_{t} r\right) d r=\frac{q}{\pi \Sigma_{t}}\left[-K I_{3}\left(\Sigma_{t} r\right)\right]_{r=0}^{r=+\infty}$
Given that $K I_{3}(0)=\frac{\pi}{4}$ and $K I_{3}(+\infty)=0$, for a source that fills up half space, the current is simply given by:

$$
J=\frac{q}{4 \Sigma_{t}}
$$

An infinitely-absorbing screen is placed at a distance $d$ (its thickness no longer matters for the calculation) with a cylindrical geometry such that radially, it has a solid angle $2 \theta_{0}$ and axially, it has a height of $2 h$ in the half "source-space." Therefore, all neutrons that are incident from the space shadowed by the screen cannot reach the detector position. The current from the shaded zone, i.e. the region hidden by the screen, is calculated as previously (using the same notations) (Fig. 14.13):

$$
J_{\text {shadow }}^{\text {cylindrical }}=q \int_{\theta=-\theta_{0}}^{\theta=+\theta_{0}} \int_{r=d}^{r=+\infty} r d r d \theta r \cos \theta \int_{z=-h}^{z=+h} \frac{e^{-\Sigma_{l} R}}{4 \pi R^{3}} d z
$$

If the cylinder is of infinite height, the calculation may be simplified to:

$$
\begin{aligned}
J_{\text {shadow }}^{\text {cylindrical }} & =\frac{q}{2 \pi} \int_{\theta=-\theta_{0}}^{\theta=+\theta_{0}} \int_{r=d}^{r=+\infty} d r d \theta \cos \theta K I_{2}\left(\Sigma_{t} r\right)=\frac{q}{2 \pi \Sigma_{t}}[\sin \theta]_{-\theta_{0}}^{+\theta_{0}} \int_{r=d}^{r=+\infty} K I_{2}\left(\Sigma_{t} r\right) d r \\
& =\frac{q}{\pi \Sigma_{t}} \sin \theta_{0} K I_{3}\left(\Sigma_{t} d\right)
\end{aligned}
$$

Fig. 14.13 Shadowing effect owing to a flat screen (the notations are the same for a cylindrical screen centered about the detector position)


For the finite cylindrical portion, the Dancoff factor is equal to:

$$
C^{\text {cylindrical }} \equiv \frac{J_{\text {shadow }}^{\text {cylindical }}}{J}=\frac{\frac{q}{\pi \Sigma_{t}} \sin \theta_{0} K I_{3}\left(\Sigma_{t} d\right)}{\frac{q}{4 \Sigma_{t}}}=\frac{\sin \theta_{0} K I_{3}\left(\Sigma_{t} d\right)}{\pi}
$$

$C$ is the relative decrease of the current due to the shadowing effect. It can be considered as the effect due to a decrease in the available surface. It is equivalent to a "shaded" surface for an object with an incident neutron on its surface, multiplied by the reduction coefficient $1-C$. This calculation is valid only for a given point of the target surface area. In real cases, $C$ is averaged over the points of the target surface.

The case of a slab of width $2 a$ and height $2 h$ complicates the range of the integral in $r$ :

$$
J_{\text {shadow }}^{\text {slab }}=q \int_{\theta=-\tan ^{-1} \frac{a}{d}}^{\theta=+\tan ^{-1} \frac{a}{d}} r=\frac{d}{\cos \theta} \quad r d r d \theta r \cos \theta \int_{z=-h}^{r=+\infty} \frac{e^{-\Sigma_{t} R}}{4 \pi R^{3}} d z
$$

This equation can be simplified for an infinite slab in $z$ :

$$
\begin{aligned}
J_{\text {shadow }}^{\text {Slab }} & =\frac{q}{2 \pi} \int_{\theta=-\tan -1 \frac{a}{d}}^{\theta=+\tan ^{-1 \frac{a}{d}}} d \theta \cos \theta \int_{r=\frac{d}{\cos \theta}}^{r=+\infty} K I_{2}\left(\Sigma_{t} r\right) d r \\
& =\frac{q}{2 \pi \Sigma_{t}} \int_{\theta=-\tan ^{-1} \frac{a}{d}}^{\theta=+\tan ^{-1} \frac{a}{d}} K I_{3}\left(\Sigma_{t} \frac{d}{\cos \theta}\right) \cos \theta d \theta
\end{aligned}
$$

Assuming that the slab now has an infinite width, using the parity of the BickleyNayler function $\mathrm{KI}_{3}(x)$, the following equation is obtained:

$$
J_{\text {shadow }}^{\text {slab }}=\frac{q}{2 \pi \Sigma_{t}} \int_{\theta=-\frac{\pi}{2}}^{\theta=+\frac{\pi}{2}} K I_{3}\left(\Sigma_{t} \frac{d}{\cos \theta}\right) \cos \theta d \theta=\frac{q}{\pi \Sigma_{t}} \int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{3}\left(\Sigma_{t} \frac{d}{\cos \theta}\right) \cos \theta d \theta
$$

Integrating by parts, the equation becomes:

$$
\frac{\pi \Sigma_{t}}{q} J_{\text {shadow }}^{\text {slab }}=\underbrace{\left[K I_{3}\left(\frac{\Sigma_{t} d}{\cos \theta}\right) \sin \theta\right]_{\theta=0}^{\theta=+\frac{\pi}{2}}}_{0}-\int_{\theta=0}^{\theta=+\frac{\pi}{2}}-K I_{2}\left(\frac{\Sigma_{t} d}{\cos \theta}\right) \frac{\Sigma_{t} d}{\cos ^{2} \theta} \sin ^{2} \theta d \theta
$$

With $\tau=\frac{\Sigma_{t} d}{\cos \theta}, d \tau=\frac{\Sigma_{t} d}{\cos ^{2} \theta} \sin \theta d \theta$, it is transformed as follows:

$$
\frac{\pi \Sigma_{t}}{q} J_{\text {shadow }}^{\text {slab }}=\int_{\tau=\Sigma_{l} d}^{\tau=+\infty} K I_{2}(\tau) \sin \theta d \tau=\int_{\tau=\Sigma_{l} d}^{\tau=+\infty} K I_{2}(\tau) \sqrt{1-\frac{\left(\Sigma_{t} d\right)^{2}}{\tau^{2}} d \tau}
$$

This equation introduces a particular integral of the Bickley-Nayler function:

$$
\begin{aligned}
& I_{n, m}\left(\Sigma_{t} d\right)=\int_{\tau=\Sigma_{l} d}^{\tau=+\infty} K I_{n}(\tau) \frac{\left(\tau^{2}-\left(\Sigma_{t} d\right)^{2}\right)^{m}}{\tau^{n-1}} d \tau \\
& =\int_{\tau=\Sigma_{t} d}^{\tau=+\infty}\left(\int_{w=0}^{w=+\infty} \frac{e^{-\tau c h w}}{c h^{n} w} d w\right) \frac{\left(\tau^{2}-\left(\Sigma_{t} d\right)^{2}\right)^{m}}{\tau^{n-1}} d \tau
\end{aligned}
$$

Let us integrate this function by setting $x=\frac{\tau c h w}{\Sigma_{t} d}$ and $y=\frac{\tau}{\Sigma_{l} d c h w}$, then:

$$
I_{n, m}\left(\Sigma_{t} d\right)=\frac{\left(\Sigma_{t} d\right)^{2 m-n+2}}{2} \int_{x=1}^{x=+\infty} e^{-\Sigma_{t} d x} x^{-n+\frac{1}{2}} d x \int_{y=\frac{1}{x}}^{y=x} \frac{(x y-1)^{m}}{\sqrt{x-y}} d y
$$

The integral over $y$ can be computed by setting:

$$
\begin{gathered}
p=\frac{x y-1}{x^{2}-1} \text { therefore } y=\frac{p\left(x^{2}-1\right)+1}{x} \quad \text { and } \quad d y=\frac{x^{2}-1}{x} d p \\
\int_{y=\frac{1}{x}}^{y=x} \frac{(x y-1)^{m}}{\sqrt{x-y}} d y=\frac{\left(x^{2}-1\right)^{m+\frac{1}{2}}}{\sqrt{x}} \int_{p=0}^{p=1} \frac{p^{m}}{\sqrt{(1-p)}} d p \equiv \frac{\left(x^{2}-1\right)^{m+\frac{1}{2}}}{\sqrt{x}} \beta\left(m+1, \frac{1}{2}\right)
\end{gathered}
$$

From which we introduce the beta function, with the real factorial function: $\beta(z, w) \equiv \frac{\Gamma(z) \Gamma(w)}{\Gamma(z+w)}=\int_{t=0}^{t=1} t^{z-1}(1-t)^{w-1} d t$ (Abramowitz and Stegun 1972, p. 258).

Thus:

$$
I_{n, m}\left(\Sigma_{t} d\right)=\frac{\left[\Sigma_{t} d\right]^{2 m-n+2}}{2} \int_{x=1}^{x=+\infty} e^{-\Sigma_{t} d x} x^{-n+\frac{1}{2}} \frac{\left(x^{2}-1\right)^{m+\frac{1}{2}}}{\sqrt{x}} \beta\left(m+1, \frac{1}{2}\right) d x
$$

In the case being considered, the following is obtained:

$$
I_{2, \frac{1}{2}}\left(\Sigma_{t} d\right)=\frac{\Sigma_{t} d}{2} \int_{x=1}^{x=+\infty} e^{-\Sigma_{t} d x} x^{-2}\left(x^{2}-1\right) \underbrace{\beta\left(\frac{3}{2}, \frac{1}{2}\right)}_{\frac{\pi}{2}} d x=\frac{\pi d}{4} \int_{x=1}^{x=+\infty} e^{-\Sigma_{l} d x}\left(1-\frac{1}{x^{2}}\right) d x
$$

The following exponential integral is reached: $E_{n}(x)=\int_{t=1}^{t=+\infty} \frac{e^{-x t}}{t^{n}} d t$
This integral can be calculated directly using $E_{2}(x)$, but it is more judicious to proceed by integrating by parts with $u=1-\frac{1}{x^{2}}$ and $v^{\prime}=e^{-\Sigma_{t} d x}$, giving:

$$
I_{2, \frac{1}{2}}(d)=\frac{\pi \Sigma_{t} d}{4}(\underbrace{\left[-\frac{e^{-\Sigma_{t} d x}}{\Sigma_{t} d}\left(1-\frac{1}{x^{2}}\right)\right]_{1}^{+\infty}}_{0}+\frac{2 E_{3}\left(\Sigma_{t} d\right)}{\Sigma_{t} d})=\frac{\pi E_{3}\left(\Sigma_{t} d\right)}{2}
$$

Finally:

$$
J_{\text {shadow }}^{\text {slab }}=\frac{q E_{3}\left(\Sigma_{t} d\right)}{2 \Sigma_{t}} \quad \text { and } \quad C_{\text {shadow }}^{\text {slab }}=\frac{J_{\text {shadow }}^{\text {slab }}}{J}=\frac{\frac{q E_{3}\left(\Sigma_{t} d\right)}{2 \Sigma_{t}}}{\frac{q}{4 \Sigma_{t}}}=2 E_{3}\left(\Sigma_{t} d\right)
$$

It is extremely interesting to note that even if a hard integration method is employed for the cylindrical case, the expected exponential integral is obtained in plane geometry. Using these mathematical tools, other cases can be integrated for problems with shadowing effects (for instance, the historical problem of Dancoff and Ginsburg: the shadow of a cylindrical rod on another cylindrical rod).

The case of a moderating cylinder is also very interesting. Let us consider an axially infinite cylinder of radius $a$ filled with moderator. We can calculate the shadowing effect with respect to a detector position located at the surface of that cylinder (Fig. 14.14).

Fig. 14.14 Cylinder with moderator


No neutrons can reach the zone located outside the cylinder with the moderator (the zone is denoted as $\cap c y l i n d e r$ ). The current unable to reach the detector position is given by:

$$
\begin{aligned}
J_{\text {shadow }}^{\cap \text { cylinder }} & =\frac{q}{2 \pi} \int_{\theta=-\frac{\pi}{2}}^{\theta=+\frac{\pi}{2}} \int_{r=2 a \cos \theta}^{r=+\infty} r d r d \theta \frac{\cos \theta}{r} K I_{2}\left(\Sigma_{t} r\right) \\
& =\frac{q}{2 \pi \Sigma_{t}} \int_{\theta=-\frac{\pi}{2}}^{\theta=+\frac{\pi}{2}} K I_{3}\left(\Sigma_{t} 2 a \cos \theta\right) \cos \theta d \theta
\end{aligned}
$$

The corresponding Dancoff factor is:

$$
\begin{aligned}
C_{\text {shadow }}^{\text {ncylinder }} & =\frac{J_{\text {shadow }}^{\cap \text { cylinder }}}{J}=\frac{\frac{q}{2 \pi \Sigma_{t}} \int_{\theta=-\frac{\pi}{2}}^{\theta=+\frac{\pi}{2}} K I_{3}\left(\Sigma_{t} 2 a \cos \theta\right) \cos \theta d \theta}{\frac{q}{4} \Sigma_{t}} \\
& =\frac{4}{\pi} \int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{3}\left(\Sigma_{t} 2 a \cos \theta\right) \cos \theta d \theta
\end{aligned}
$$

The integral of function $K I_{3}$ is split through successive integrations by parts:

$$
\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{3}\left(\Sigma_{t} 2 a \cos \theta\right) \cos \theta d \theta=\underbrace{\left[K I_{3}\left(\Sigma_{t} 2 a \cos \theta\right) \sin \theta\right]_{0}^{\frac{\pi}{2}}}_{K I_{3}(0)-\frac{\pi}{4}}-\Sigma_{t} 2 a \int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{2}\left(\Sigma_{t} 2 a \cos \theta\right) \sin ^{2} \theta d \theta
$$

Hence:

$$
\frac{\pi}{8 \Sigma_{t} a}\left(1-C_{\text {shadow }}^{\text {ncylinder }}\right)=\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{2}\left(\Sigma_{t} 2 a \cos \theta\right) \sin ^{2} \theta d \theta=
$$

Using the recurrence formula for the Bickley-Nayler functions, we obtain:

$$
r K I_{r+1}(z)=-z K I_{r}(z)+(r-1) K I_{r-1}(z)+z K I_{r-2}(z)
$$

Therefore:

$$
K I_{2}(z)=-z K I_{2}(z)+z K I_{-1}(z)=-z K I_{2}(z)+z K_{1}(z)
$$

Since $K I_{-n}(z)=(-1)^{n} \frac{d^{n} K_{0}(z)}{d z^{n}}$ (Abramowitzt and Stegun 1972, p. 258),
i.e.:

$$
K I_{-1}(z)=-\frac{d K_{0}(z)}{d z}=K_{1}(z) .
$$

Hence:
$\frac{\pi}{8 \Sigma_{t} a}\left(1-C_{\text {shadow }}^{\text {กcylinder }}\right)=\int_{\theta=0}^{\theta=+\frac{\pi}{2}}\left(K_{1}\left(\Sigma_{t} 2 a \cos \theta\right)-K I_{1}\left(\Sigma_{t} 2 a \cos \theta\right)\right) \Sigma_{t} 2 a \cos \theta \sin ^{2} \theta d \theta$
The two integrals are evaluated by integrating by parts. For the first integral, let:

$$
\begin{aligned}
u^{\prime}=K_{1}\left(\Sigma_{t} 2 a \cos \theta\right) \Sigma_{t} 2 a \sin \theta \quad \text { and } & v=\cos \theta \sin \theta=\frac{\sin 2 \theta}{2}: \\
\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K_{1}\left(\Sigma_{t} 2 a \cos \theta\right) \Sigma_{t} 2 a \cos \theta \sin ^{2} \theta d \theta & =\underbrace{\left[K_{1}\left(\Sigma_{t} 2 a \cos \theta\right) \cos \theta \sin \theta\right]_{0}^{\frac{\pi}{2}}}_{0} \\
& -\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K_{0}\left(\Sigma_{t} 2 a \cos \theta\right) \cos 2 \theta d \theta
\end{aligned}
$$

The second integral is obtained by setting $u^{\prime}=\cos \theta \sin ^{2} \theta$ and $v=\Sigma_{t} 2 a K I_{1}\left(\Sigma_{t} 2 a \cos \theta\right)$ :

$$
\begin{aligned}
\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{1}\left(\Sigma_{t} 2 a \cos \theta\right) \Sigma_{t} 2 a \cos \theta \sin ^{2} \theta d \theta= & \underbrace{\left[\Sigma_{t} 2 a K I_{1}\left(\Sigma_{t} 2 a \cos \theta\right) \frac{\sin ^{3} \theta}{3}\right]_{0}^{\frac{\pi}{2}}}_{\frac{\Sigma_{1} a \pi}{3}} \\
& -\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{0}\left(\Sigma_{t} 2 a \cos \theta\right)\left(\Sigma_{t} 2 a\right)^{2} \sin \theta \frac{\sin ^{3} \theta}{3} d \theta
\end{aligned}
$$

Noting that $\sin ^{4} \theta=\frac{3}{8}-\frac{1}{2} \cos 2 \theta+\frac{1}{8} \cos 4 \theta$, the following equation may be deduced:

$$
\begin{aligned}
& \int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{1}\left(\Sigma_{t} 2 a \cos \theta\right) \Sigma_{t} 2 a \cos \theta \sin ^{2} \theta d \theta=\frac{\Sigma_{t} a \pi}{3} \\
& -\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K I_{0}\left(\Sigma_{t} 2 a \cos \theta\right)\left(\Sigma_{t} 2 a\right)^{2}\left(\frac{1}{8}-\frac{1}{6} \cos 2 \theta+\frac{1}{24} \cos 4 \theta\right) d \theta \\
& \frac{\pi}{8 \Sigma_{t} a}\left(1-C_{\text {shadow }}^{\text {ncylinder }}\right)=-\frac{\Sigma_{t} a \pi}{3} \\
& \quad+\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K_{0}\left(\Sigma_{t} 2 a \cos \theta\right)\left(-\cos 2 \theta+\frac{\left(\Sigma_{t} a\right)^{2}}{2}-\frac{2\left(\Sigma_{t} a\right)^{2}}{3} \cos 2 \theta+\frac{\left(\Sigma_{t} a\right)^{2}}{6} \cos 4 \theta\right) d \theta
\end{aligned}
$$

Using the next equation (Watson 1980, p. 441):

$$
\int_{\theta=0}^{\theta=+\frac{\pi}{2}} K_{0}(2 z \cos \theta) \cos (2 n \theta) d \theta=(-1)^{n} \frac{\pi}{2} I_{n}(z) K_{n}(z)
$$

The equation thus obtained is:

$$
\begin{aligned}
\frac{\pi}{8 \Sigma_{t} a}\left(1-C_{\text {shadow }}^{\text {ncylinder }}\right)= & -\frac{\Sigma_{t} a \pi}{3}+\frac{\left(\Sigma_{t} a\right)^{2} \pi}{2} I_{0}\left(\Sigma_{t} a\right) K_{0}\left(\Sigma_{t} a\right) \\
& +\left(1+\frac{2\left(\Sigma_{t} a\right)^{2}}{3}\right) \frac{\pi}{2} I_{1}\left(\Sigma_{t} a\right) K_{1}\left(\Sigma_{t} a\right)+\frac{\left(\Sigma_{t} a\right)^{2} \pi}{6} I_{2}\left(\Sigma_{t} a\right) K_{2}\left(\Sigma_{t} a\right)
\end{aligned}
$$

The recurrence relations for the Bessel functions are next used (Abramowitz and Stegun 1972, p. 376), such that:

$$
\left\{\begin{array}{l}
I_{n-1}(x)-I_{n+1}(x)=\frac{2 n}{x} I_{n}(x) \\
e^{i(n-1) \pi} K_{n-1}(x)-e^{i(n+1) \pi} K_{n+1}(x)=\frac{2 n}{x} e^{i n \pi} K_{n}(x)
\end{array}\right.
$$

and, the term $I_{2}\left(\Sigma_{t} a\right) K_{2}\left(\Sigma_{t} a\right)=\left(I_{0}\left(\Sigma_{t} a\right)-\frac{2}{\Sigma_{t} a} I_{1}\left(\Sigma_{t} a\right)\right)\left(K_{0}\left(\Sigma_{t} a\right)+\frac{2}{\Sigma_{t} a} K_{1}\left(\Sigma_{t} a\right)\right)$ is degenerated.

Finally:

$$
\begin{aligned}
\frac{1}{2 \Sigma_{t} a}\left(1-C_{\text {shadow }}^{\cap \text { cylinder }}\right)= & -\frac{4 \Sigma_{t} a}{3}+\frac{4\left(\Sigma_{t} a\right)^{2}}{3} I_{0}\left(\Sigma_{t} a\right) K_{0}\left(\Sigma_{t} a\right) \\
& +2\left(\frac{1}{3}+\frac{2\left(\Sigma_{t} a\right)^{2}}{3}\right) I_{1}\left(\Sigma_{t} a\right) K_{1}\left(\Sigma_{t} a\right) \\
& +\frac{2 \Sigma_{t} a}{3} I_{0}\left(\Sigma_{t} a\right) K_{1}\left(\Sigma_{t} a\right)-I_{1}\left(\Sigma_{t} a\right) K_{0}\left(\Sigma_{t} a\right) \\
= & \frac{2 \Sigma_{t} a}{3}\left\{2\left[\Sigma_{t} a\left(I_{1}\left(\Sigma_{t} a\right) K_{1}\left(\Sigma_{t} a\right)+I_{0}\left(\Sigma_{t} a\right) K_{0}\left(\Sigma_{t} a\right)\right)-1\right]\right. \\
& \left.+\frac{I_{1}\left(\Sigma_{t} a\right) K_{1}\left(\Sigma_{t} a\right)}{\Sigma_{t} a}-I_{1}\left(\Sigma_{t} a\right) K_{0}\left(\Sigma_{t} a\right)+I_{0}\left(\Sigma_{t} a\right) K_{1}\left(\Sigma_{t} a\right)\right\}
\end{aligned}
$$

This final equation has been rewritten only to illustrate an exact form of equation 28 from page 33 of (Case et al. 1953), which gives the leakage probability for an infinite cylinder $P_{0}$ (denoted as $P_{V S, 0}$ and given in a previous chapter without any derivation). It should be noted that the original equation contained a few errors which were thus corrected in this work. Furthermore, it is worth pointing out that this result was historically obtained by D. Inglis in 1942 at Los Alamos (cited by Case et al.) without the use of the $K I$ functions. The calculation illustrated here was made by I. Carlvik and B. Pershagen in 1959.

Thus, several integration techniques for cylindrical problems have been illustrated for dealing with numerous cases of extruded geometries along a given axis, be it vertical (PWR, fast reactors, etc.) or horizontal (heavy water reactors, some $U N G G)$. In the case of fuel lattices, angular integration problems will rise along with the "non-shadowing factor" for each pin with respect to one another-the same difficulty arises in thermal radiative transfer. The analytical calculation is extremely laborious and can be usefully replaced by ray tracing in the considered geometry.

### 14.3.3.4 Impact of the Dancoff Factor on Resonant Absorption

This factor is clearly important for cases of packed lattices. It impacts the mean chord value $<\ell\rangle=4 V / S$, which appears in the calculation of the effective resonance integral:

$$
<\ell>_{\text {Danc }}=\frac{<\ell>}{1-C}
$$

The term $N_{U}<\ell>_{\text {Danc }}$ also appears for the Narrow Resonance Infinite Mass (NRIM) method, through the Wigner rational approximation of the leakage probability, discussed in earlier chapters, with the usual notations:

$$
I=I_{\infty} \sqrt{\frac{\beta}{1+\beta}} \quad \text { with }: \beta \equiv \frac{\sigma_{p}+\frac{1}{N_{U}<\ell>_{\text {Danc }}}}{\sigma_{t}} \frac{\Gamma}{\Gamma_{\gamma}}
$$

The sensitivity of the resonance integral to the Dancoff factor is calculated as ${ }^{22}$ :

$$
\frac{C}{I} \frac{\partial I}{\partial C}=\frac{C}{2(1-C)} \frac{\frac{\sigma_{p}}{\sigma_{t}}-\beta}{\beta(1+\beta)}
$$

for which the maximum value is reached for $\beta=\frac{\sigma_{p}}{\sigma_{t}}+\sqrt{\frac{\sigma_{p}}{\sigma_{t}}\left(1+\frac{\sigma_{p}}{\sigma_{t}}\right) \approx \sqrt{\frac{\sigma_{p}}{\sigma_{t}}}}$.
For this maximum value, the following equations hold:

$$
\langle\ell\rangle_{\text {Danc }}=\frac{\langle\ell\rangle}{1-C} \approx \frac{1}{N_{U \sqrt{\sigma_{p} \sigma_{t}}}} \quad \text { and } \quad\left(\frac{C}{I} \frac{\partial I}{\partial C}\right)=-\frac{C}{2(1-C)}
$$

As the Dancoff factor tends towards 1 , the impact on the resonance integral becomes significant.

### 14.3.3.5 Extension to Pin Lattices

The multi-cell approach may be extended to lattices of regular cells with some cells being differentiated (e.g. guide tubes) using $S_{i j}{ }^{23}$ method. Let us consider two cells $A$ and $B$. Using the inner probabilities of the cells, the following can be written:

$$
P_{i \in A, j \in B}=P_{i j}^{+} \delta_{A, B}+P_{i \in A, S}^{+} Q_{A, B} P_{S, j \in B}^{+}
$$

[^296]The Kronecker delta $\delta_{A, B}$ equals 1 if $A=B$ and 0 otherwise. Multiplied by $P_{i j}^{+}$, it corresponds to the first-collision probability of two zones within a cell.
$Q_{A, B}$ is the non-collided incident current in cell $B$ for a neutron leaving cell $A$ (with probability $P_{i \in A, S}^{+}$) uniformly and isotropically. This coefficient can be higher than 1 and should not be confused with a probability. It corresponds to the mean number of times that a neutron emitted in cell $A$ crosses cell $B$ before undergoing its first collision in cell $B$. In Fig. 14.15, $Q_{A, B}$ is equal to 3 .

Let $S_{A B}$ be the probability that an outgoing neutron from $A$ directly enters the adjacent cell $B$. Indeed, $S_{A B}$ can be calculated as the ratio between the common boundaries of cells $A$ and $B$ after the cylindrical approximation to outer surface of cell $A$.

In Fig. 14.16, the calculation of $S_{A B}$ with the Roth hypothesis leads to: $S_{A B}=1$, $S_{A A}=0, S_{A B A}=\frac{1}{8}, S_{B B}=\frac{7}{8}$. It can be seen that corner cells have the same weight as cells on the sides due to the cylindrical approximation. The complementary relation allows the normalization of $S_{i j}$ :

$$
\sum_{j} S_{i j}=1
$$

The reciprocity relation for $P_{i j}$ values imposes an identical relation at $S_{i j}$ :

$$
\sum_{i \in A} \text { Surface }_{A} S_{i B}=\sum_{j \in B} \text { Surface }_{B} S_{j A}
$$

This is simply given as follows, with $n_{A}$ being the number of cells $A$ and $n_{B}$ that of $B$ :

$$
n_{A} \text { Surface }_{A} S_{A B}=n_{B} \text { Surface }_{B} S_{B A}
$$

In the end, the neutron has a probability $S_{A B}$ of entering cell $B$ when coming from $A$. Otherwise, it enters cell $D$ and it has a probability $P_{S S, D}^{+}$of crossing that cell without colliding. It can cross cell $B Q_{D B}$ times before finally colliding in $B$ :

Fig. 14.15 Crossing of cells


Fig. 14.16 Pattern with nine cells, with a different cell at the center


$$
Q_{A B}=S_{A B}+\sum_{D} S_{A D} P_{S S, D}^{+} Q_{D B}
$$

Evaluating all the $S_{i j}$ values and the calculation of all the $P_{S S, i}^{+}$for the cells lead to a linear system with respect to $Q_{i j}$ that is easily solved. For the case of a lattice with identical cells, the following formalism is deduced, as with an infinite lattice:

$$
Q_{A A}=\frac{1}{1-P_{S S, A}^{+}} \quad \text { and } \quad P_{i j, A}=P_{i j, A}^{+}+\frac{P_{i S, A}^{+} P_{S j, A}^{+}}{1-P_{S S, A}^{+}}
$$

It should be emphasized that this method allows for approximate spatial coupling of cells since each $A$ cell ends up with the same flux. Optimization is required to group cells having similar physical traits such as fuel cells with a common boundary with a guide tube cell or cells on the assembly boundary that are impacted by the inter-assembly water gap. Further, the cylindrical approximation has been significantly improved over the years. The first improvement consisted in differentiating the currents for the four interfaces of a $P W R$ cell (Roth 4 model). In addition, the cylindrical approximation effect can be decreased by using isotropic or linear interface currents ( $U P 0$ or $U P 1$ approximation of the APOLLO2 code). Finally, the probabilities can be calculated on the exact 2D geometry using the sweeping and tracking techniques discussed in the Transport chapter. Moreover, there have been recent attempts to use collision probability methods $P_{i j}$ on 3D geometries; these calculations are extremely costly but may become widespread with the advent of massive parallel calculations.

### 14.3.4 Carlvik Rational Approximation

(Stamm'ler and Abbate 1983, p. 301)

In 1964, Carlvik proposed ${ }^{24}$ an approximation of the fuel-fuel collision probability for a single pin $P_{f, f}^{+}$using a rational function for the optical path $X=4 V_{f} \Sigma_{t, f} / S$, where $V_{c}$ is the fuel volume, $\Sigma_{t, c}$ is the fuel total cross section, and $S$ is the fuel surface area:

Carlvik rational approximation:

$$
\begin{equation*}
P_{f, f}^{+} \approx \frac{B X}{X+A_{1}}+\frac{(1-B) X}{X+A_{2}} \quad \text { with } B=2, A_{1}=2, A_{2}=3 \tag{14.6}
\end{equation*}
$$

This approximation forms part of the more general rational approximations (Stamm'ler and Abbate 1983, p. 297; Ferziger and Zweifel 1966, p. 117), where the probability $P_{f, f}^{+}$is written as:

$$
P_{f, f}^{+}=X \sum_{n} \frac{B_{n}}{X+A_{n}} \quad \text { with } \sum_{n} B_{n}=1
$$

The Wigner rational approximation which models the non-collided leakage probability by $P_{V S, 0}=\frac{1}{1+\Sigma_{t}\langle R\rangle}=\frac{1}{1+X}$, leads to $P_{f, f}^{+}=1-P_{V S, 0}=\frac{X}{1+X}$, for which precision can be improved using the Bell factor discussed in Chap. 5: $P_{f, f}^{+}=\frac{X}{a_{\text {Bell }}+X}$

Such approximations enable calculation of the resonance integral in a heterogeneous medium by substituting it with a combination of homogeneous medium integrals.

It was seen earlier that the probability of collision inside the fuel, $P_{f, f}$, may be given by the Dancoff formula (Eq. (14.5) with $P_{c c}$ and $j=c$ ). It can be written here using $F$, the cell surface, rather than the fuel surface (since the same reasoning underpinning this equation with $S$ is also valid for $F$ ):

$$
P_{f, f}=P_{f, f}^{+}+\frac{P_{f, F}^{+} P_{F, f}^{+}}{1-P_{F, F}^{+}}
$$

The probability $1-P_{F, F}^{+}$that a neutron, entering through the cell boundary isotropically, will interact inside that cell can be decomposed into:

$$
1-P_{F, F}^{+}=P_{F, S}^{+} P_{S, f}^{+}+P_{F, S}^{+}\left(1-P_{S, F}^{+}\right)\left(1-P_{S, f}^{+}\right)+\sum_{i \neq f} P_{F, i}^{+}
$$

where $P_{F, S}^{+}$is the probability of an isotropically incoming neutron in the cell reaching the fuel surface without collision, $P_{S, f}^{+}$is the probability of an isotropically

[^297]incoming neutron in the fuel undergoing its first collision inside the fuel, $P_{S, F}^{+}$is the probability of an isotropically outgoing neutron from the fuel reaching the cell boundary. The term $P_{F, S}^{+} P_{S, f}^{+}$represents neutrons traveling from the cell boundary and colliding for the first time inside the fuel. The term $P_{F, S}^{+}\left(1-P_{S, F}^{+}\right)\left(1-P_{S, f}^{+}\right)$ corresponds to the collisions of neutrons crossing the fuel (their proportion being $1-P_{S, f}^{+}$). Finally, the term $\sum_{i \neq f} P_{F, i}^{+}$represents the contributions of neutrons that do not reach the fuel (but reach other media such as the cladding or the moderator). With the reciprocity relation:
$$
F P_{F, S}^{+}=S P_{S, F}^{+}
$$

Moreover:

$$
P_{F, f}^{+}=\frac{4 V_{f} \Sigma_{l, f}}{F}\left(1-P_{f, f}^{+}\right)=X\left(1-P_{f, f}^{+}\right)
$$

Thus:

$$
1-P_{F, F}^{+}=\frac{S}{F}\left(P_{S, F}^{+}\right)^{2} X\left(1-P_{f, f}^{+}\right)+P_{F, S}^{+}\left(1-P_{S, F}^{+}\right)+\sum_{i \neq f} P_{F, i}^{+}
$$

Since:

$$
P_{F, f}^{+}=\frac{4 V_{f} \Sigma_{l, f}}{F} P_{f, F}^{+}=\frac{X S}{F} P_{f, F}^{+}=\frac{X S}{F}\left(1-P_{f, f}^{+}\right) P_{S, F}^{+}, \text {the Dancoff rela- }
$$ tion is finally expressed as:

$$
\begin{aligned}
P_{f, f} & =P_{f, f}^{+}+\frac{P_{f, F}^{+} P_{F, f}^{+}}{1-P_{F, F}^{+}} \\
& =P_{f, f}^{+}+\frac{\frac{X S}{F}\left(P_{S, F}^{+}\right)^{2}\left(1-P_{f, f}^{+}\right)^{2}}{\frac{S}{F}\left(P_{S, F}^{+}\right)^{2} X\left(1-P_{f, f}^{+}\right)+P_{F, S}^{+}\left(1-P_{S, F}^{+}\right)+\sum_{i \neq f} P_{F, i}^{+}}
\end{aligned}
$$

The previous equation can be simplified by setting:

$$
\begin{aligned}
& K=\frac{P_{F, S}^{+}\left(1-P_{S, F}^{+}\right)+\sum_{i \neq f} P_{F, i}^{+}}{\frac{S}{F}\left(P_{S, F}^{+}\right)^{2}}, \text { hence: } \\
& P_{f, f}= P_{f, f}^{+}+\frac{X\left(1-P_{f, f}^{+}\right)^{2}}{X\left(1-P_{f, f}^{+}\right)+K}
\end{aligned}
$$

Inserting this equation in the Carlvik rational approximation (Eq. 14.6) expressed under the form:

$$
\left\{\begin{array}{l}
P_{f, f}^{+}=\frac{B X}{X+A_{1}}+\frac{(1-B) X}{X+A_{2}}=\frac{X^{2}+\left[B\left(A_{2}-A_{1}\right)+A_{1}\right] X}{\left(X+A_{1}\right)\left(X+A_{2}\right)}=\frac{X^{2}+(S-C) X}{\left(X+A_{1}\right)\left(X+A_{2}\right)} \\
1-P_{f, f}^{+}=1-\frac{X^{2}+(S-C) X}{\left(X+A_{1}\right)\left(X+A_{2}\right)}=\frac{X^{2}+S X+P-\left(X^{2}+(S-C) X\right)}{\left(X+A_{1}\right)\left(X+A_{2}\right)}=\frac{C X+P}{\left(X+A_{1}\right)\left(X+A_{2}\right)}
\end{array}\right.
$$

with $S=A_{1}+A_{2}$ being the sum of the coefficients in Carlvik's formula and $P=A_{1}$. $A_{2}$ their product. Let us define $\left(X+A_{1}\right)\left(X+A_{2}\right) \equiv X^{2}+S X+P, C \equiv B\left(A_{2}-A_{1}\right)+A_{1}$. Hence, $P_{f, f}$ can be written as a rational approximation:

$$
P_{f, f}=\frac{\beta X}{X+\alpha_{1}}+\frac{(1-\beta) X}{X+\alpha_{2}}=\frac{X^{2}+\left[\beta\left(\alpha_{2}-\alpha_{1}\right)+\alpha_{1}\right] X}{\left(X+\alpha_{1}\right)\left(X+\alpha_{2}\right)}=\frac{X^{2}+\lambda X}{X^{2}+s X+p}
$$

with $s=\alpha_{1}+\alpha_{2}$ and $p=\alpha_{1} . \alpha_{2}$. Mathematical calculations lead to equating two polynomials of degree 5 after reducing two fractions to the same denominator:

$$
\frac{X^{2}+\lambda X}{\left(X+\alpha_{1}\right)\left(X+\alpha_{2}\right)}=\frac{X^{2}+(S-C) X}{\left(X+A_{1}\right)\left(X+A_{2}\right)}+\frac{X \frac{(C X+P)^{2}}{\left(X+A_{1}\right)^{2}\left(X+A_{2}\right)^{2}}}{X \frac{(C X+P)}{\left(X+A_{1}\right)\left(X+A_{2}\right)}+K}
$$

which after some algebraic calculations leads to:

$$
\begin{aligned}
& {\left[\begin{array}{l}
(K+C) X^{5}+ \\
(P+K S+(S+\lambda)(K+C)) X^{4}+ \\
(K P+(S+\lambda)(P+K S)+(P+\lambda S)(K+C)) X^{3}+ \\
{[(S+\lambda) K P+(P+\lambda S)(P+K S)+P \lambda(K+C)] X^{2}+} \\
(P \lambda(P+K S)+K P(P+\lambda S)) X+ \\
P^{2} \lambda K
\end{array}\right]} \\
& =\left[\begin{array}{l}
{[K+C] X^{5}+} \\
{\left[C^{2}+P+K S+(K+C)(S-C)+s[K+C]\right] X^{4}+} \\
{\left[p[K+C]+s\left[C^{2}+P+K S+(K+C)(S-C)\right]+[2 C P+K P+(P+K S)(S-C)]\right] X^{3}+} \\
{\left[p\left[C^{2}+P+K S+(K+C)(S-C)\right]+s[2 C P+K P+(P+K S)(S-C)]+\left[P^{2}+K P(S-C)\right]\right] X^{2}+} \\
s\left[P^{2}+K P(S-C)\right]+p[2 C P+K P+(P+K S)(S-C)] X X+ \\
{\left[p\left(P^{2}+K P(S-C)\right)\right]}
\end{array}\right.
\end{aligned}
$$

The first equation (coefficient of $X^{5}$ ) is trivial. The second (coefficient of $X^{4}$ ) gives:

$$
\lambda=s-\frac{K C}{K+C}
$$

This expression and the role of $\lambda$ imply that the quantities $s$ and $p$ should be sought as:

$$
s=\frac{s_{0}+s_{1} K}{K+C} \quad \text { and } \quad p=\frac{p_{0}+p_{1} K}{K+C}
$$

Inserting these equations in the linear system resulting from the equalizing of the coefficients of the polynomials gives:

$$
\left\{\begin{array}{cc}
s_{0}=p_{1} & s_{1}=\frac{P S+S C^{2}-C S^{2}}{P+C^{2}-S C} \\
p_{0}=0 & p_{1}=\frac{P\left(P S+2 S C^{2}-C S^{2}-C P-C^{3}\right)}{(S-C)\left(P+C^{2}-S C\right)}
\end{array}\right.
$$

Using the coefficients from Carlvik's formula, i.e.:

$$
\begin{aligned}
B & =3 \quad A_{1}=2 \quad A_{2}=3 \quad P=A_{1} \cdot A_{2}=6 \quad S=A_{1}+A_{2}=5 \quad C \\
& =B\left(A_{2}-A_{1}\right)+A_{1}=1
\end{aligned}
$$

The following results are obtained:

$$
s=\frac{6+5 K}{K+1} \quad p=\frac{6 K}{K+1} \quad \lambda=\frac{6+4 K}{K+1}
$$

i.e.:
$\alpha_{1}=\frac{6+5 K-\sqrt{K^{2}+36 K+36}}{2 K+2} \quad \alpha_{2}=\frac{6+5 K+\sqrt{K^{2}+36 K+36}}{2 K+2} \quad \beta=\frac{\lambda-\alpha_{1}}{\alpha_{2}-\alpha_{1}}$
All the equations from equalizing the coefficients of the polynomial of degree 5 are satisfied by these values. Using the rational approximation facilitates the calculation of the resonance integral. In the narrow resonance approximation, the resonance integral is:

$$
I_{N R}=\int_{E}\left[\left(1-P_{f, f}\right) \sigma_{t}+P_{f, f} \sigma_{p}\right] \frac{\sigma_{a}(E)}{\sigma_{t}(E)} \frac{d E}{E}
$$

$\sigma_{p}$ is the potential scattering cross section for each absorbing nuclide in the fuel. Using $P_{f, f}=\sum_{i} \frac{\beta_{i} X}{X+\alpha_{i}}=\sum_{i} \frac{\beta_{i} \sigma_{t}}{\sigma_{t}+\alpha_{i} \sigma_{e}}$, the resonance integral for a homogeneous medium is:

Resonance integral (rational approximation):

$$
\begin{equation*}
I_{N R}=\sum_{i} \beta_{i} I\left(\sigma_{p}+\alpha_{i} \sigma_{e}\right)=\sum_{i} \beta_{i} \int_{E} \frac{\sigma_{a}(E)\left(\sigma_{p}+\alpha_{i} \sigma_{e}\right)}{\sigma_{t}(E)} \frac{d E}{E} \tag{14.7}
\end{equation*}
$$

with the dilution cross section for the resonant isotope (of concentration $N_{0}$ ):

$$
\sigma_{e}=\frac{\Sigma_{e}}{N_{0}}=\frac{S_{f}}{4 V_{f} N_{0}}
$$

The mean absorption cross section integrated in energy is defined as:

$$
\sigma_{a}=\frac{\int_{E} \sigma_{a}(E) \Phi(E) d E}{\int_{E} \Phi(E) d E} \quad \text { with } \quad \Phi(E)=\left(1-P_{f, f}+\frac{\sigma_{p}}{\sigma_{t}(E)}\right) \frac{p(E)}{E}
$$

where $p(E)$ is the resonance escape probability up to energy $E$. The resonance integral can be computed in the homogeneous case and tabulated in terms of $\sigma_{p}$ (physically, the integral varies as $\sqrt{\sigma_{p}}$ ) and in terms of the fuel temperature (Doppler effect in $\sqrt{T_{f}}$. The heterogeneous case can be considered through equivalence of the resonance integral in the equivalent homogeneous case by using the mean value of the effective cross section. ${ }^{25}$ For example, the radial effect due to the absorption of ${ }_{92}^{238} U^{92}$ (rim effect) can be modeled by using a radial zoning of the fuel pin ( $M$ zones), with the zone labeled $M$ being the outer surface and corresponding to the rim effect. The effective cross section (denoted as $\sigma_{\text {inner }}$ ) for all the zones, except the rim, is calculated with the resonance integral in homogeneous medium:

$$
I_{N R}^{\mathrm{hom}}=\int_{E} \frac{\sigma_{a}(E) \sigma_{p}}{\sigma_{t}(E)} \frac{d E}{E}
$$

The mean value of the cross section for the pin $\bar{\sigma}$ is calculated using Eq. (14.7). The cross section for the rim of the pin $\sigma_{r i m}$ is computed via the calculation of a reaction rate:

$$
\sum_{i=1}^{M-1} N_{i} V_{i} \sigma_{\text {inner }} \Phi_{i}+N_{\text {rim }} V_{\text {rim }} \sigma_{\text {rim }} \Phi_{\text {rim }}=\left(\sum_{i=1}^{M-1} N_{i} V_{i}+N_{\text {rim }} V_{\text {rim }}\right) \bar{\sigma} \bar{\Phi}
$$

In this formula, the mean flux is obtained by weighting the local flux by the volumes:

$$
\bar{\Phi}=\frac{\sum_{i=1}^{M-1} V_{i} \Phi_{i}+V_{\text {rim }} \Phi_{r i m}}{\sum_{i=1}^{M-1} V_{i}+V_{\text {rim }}}
$$

[^298]It should be noted that $\sigma_{\text {rim }}$ has no physical meaning, contrary to the absorption rate $N_{\text {rim }} V_{\text {rim }} \sigma_{\text {rim }} \Phi_{\text {rim }}$. Since $\sigma_{\text {rim }}$ is inversely proportional to $V_{\text {rim }}$, this reaction rate does not depend on the size of the mesh for the rim.

### 14.3.5 Heterogeneity of the Isotopic Composition

In the case of a mixture of absorbing materials, there is a mutual self-shielding effect that is practically expressed as the fact that a neutron absorbed by a resonant nuclide can no longer be absorbed by another nuclide. This phenomenon may be modeled by calculating the resonance integral of the mixture containing $k$ resonant isotopes of concentration $N_{k}$ :

$$
\sum_{k} N_{k} I_{k}=\int_{E}\left(\sum_{k} N_{k} \sigma_{a, k}(E)\right)\left(1-P_{f, f}+\frac{\sigma_{p}}{\sigma_{t}(E)} P_{f, f}\right) \frac{d E}{E}
$$

### 14.3.6 Shadowing Effect on the Resonance Integral

In the chapter on resonant absorption, the neutron balance of a cell with fuel $c$ (for combustible in French, we do not use here usual subscript f to avoid any confusion with fission while used for cross-sections) containing a heavy nuclide $U$ and a light nuclide $m$ surrounded by a moderator $M$ was established.

$$
\left\{\begin{array}{c}
V_{c} \Sigma_{t}^{c} \Phi_{c}=V_{c}\left(1-P_{c M}\right) R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+V_{M} P_{M c} R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right] \\
V_{M} \Sigma_{t}^{M} \Phi_{M}=V_{c} P_{c M} R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right]+V_{M}\left(1-P_{M c}\right) R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right]
\end{array}\right.
$$

Using the usual notations for the slowing-down operator in the fuel:

$$
\begin{aligned}
& R_{c}\left[\Sigma_{s}^{c} \Phi_{c}\right] \equiv R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+R_{m}\left[\Sigma_{s}^{m} \Phi_{c}\right] \approx R_{U}\left[\Sigma_{s}^{U} \Phi_{c}\right]+\Sigma_{s}^{m} R_{m}\left[\Phi_{c}\right] \\
= & \frac{1}{1-\alpha_{c}} \int_{u^{\prime}=u-\varepsilon_{c}}^{u^{\prime}=u} \Sigma_{t}^{c} \Phi_{c} \frac{\Sigma_{s}^{U}}{\Sigma_{t}^{c}} e^{-\left(u-u^{\prime}\right)} d u^{\prime}+\frac{1}{1-\alpha_{m}} \int_{u^{\prime}=u-\varepsilon_{m}}^{u^{\prime}=u} \Sigma_{t}^{c} \Phi_{c} \frac{\Sigma_{s}^{m}}{\Sigma_{t}^{c}} e^{-\left(u-u^{\prime}\right)} d u^{\prime}
\end{aligned}
$$

and for the slowing down operator in the moderator:

$$
R_{M}\left[\Sigma_{s}^{M} \Phi_{M}\right] \equiv \frac{1}{1-\alpha_{c}} \int_{u^{\prime}=u-\varepsilon_{M}}^{u^{\prime}=u} \Sigma_{t}^{M} \Phi_{c} \frac{\Sigma_{s}^{M}}{\Sigma_{t}^{M}} e^{-\left(u-u^{\prime}\right)} d u^{\prime}
$$

the reciprocity relation for the probabilities is written as follows:

$$
P_{c M} V_{c} \Sigma_{t}^{c}(u)=P_{c M} V_{c}\left(\Sigma_{t}^{U}(u)+\Sigma_{s}^{m}\right)=P_{M c} V_{M} \Sigma_{t}^{M}(u) \approx P_{M c} V_{M} \Sigma_{s}^{M}(u)
$$

The effective resonance integral is expressed as:

$$
I_{\text {eff }} \equiv \int \frac{\Sigma_{a}^{U} \Phi_{c}}{\Phi_{\text {asymptotique }}} d u=\int \frac{\Sigma_{a}^{U}}{\Sigma_{t}^{c}} \Sigma_{t}^{c} \Phi_{c} d u
$$

Outside the resonances, the asymptotic flux has a $1 / E$ shape, i.e.:

$$
\Phi_{\text {asymptotic }}(E) d E=\frac{S}{\xi \Sigma_{s} E} d E \quad \text { or in lethargy } \quad \Phi_{\text {asymptotic }}(u) d u=\frac{S}{\xi \Sigma_{s}} d u
$$

By normalizing the asymptotic flux to 1 (e.g. $S=\xi \Sigma_{s}$ ) and outside resonances, the following may be written:

$$
\left\{\begin{array}{l}
\Sigma_{t}^{c} \Phi_{f} \approx\left(\Sigma_{p}^{U}+\Sigma_{s}^{m}\right) \Phi_{\text {asymptotic }}=\Sigma_{p}^{U}+\Sigma_{s}^{m} \quad \text { outside resonances } \\
\Sigma_{t}^{M} \Phi_{M} \approx \Sigma_{t}^{M} \Phi_{\text {asymptotic }} \approx \Sigma_{s}^{M} \quad \text { little absorption in moderator }
\end{array}\right.
$$

Using the Narrow Resonance (NR) approximation, the slowing-down operators can be simplified by substituting the terms $\Sigma_{t}^{c} \Phi_{c}$ and $\Sigma_{t}^{M} \Phi_{M}$ in the operators using their asymptotic expressions. Hence:

$$
\left\{\begin{array}{l}
V_{c} \Sigma_{t}^{c} \Phi_{c} \approx V_{c}\left(1-P_{c M}\right)\left(\Sigma_{p}^{U}+\Sigma_{s}^{m}\right) \underbrace{R_{c}[1]}_{1}+\underbrace{V_{M} P_{M c} \Sigma_{s}^{M}}_{\approx P_{c M} V_{c} \Sigma_{t}^{c}} \underbrace{R_{M}[1]}_{1} \\
V_{M} \Sigma_{t}^{M} \Phi_{M} \approx V_{c} P_{c M}\left(\Sigma_{p}^{U}+\Sigma_{s}^{m}\right)+V_{M}\left(1-P_{M c}\right) \Sigma_{s}^{M}
\end{array}\right.
$$

Thus:

$$
\Sigma_{t}^{c} \Phi_{c} \approx\left(1-P_{c M}\right)\left(\Sigma_{p}^{U}+\Sigma_{s}^{m}\right)+P_{c M} \Sigma_{t}^{c}
$$

which can be inserted in the effective resonance integral:

$$
I_{e f f}=\int \frac{\Sigma_{a}^{U}}{\Sigma_{t}^{c}} \Sigma_{t}^{c} \Phi_{c} d u=\underbrace{\int \frac{\Sigma_{a}^{U}}{\Sigma_{t}^{c}}\left(\Sigma_{p}^{U}+\Sigma_{s}^{m}\right) d u}_{I_{\text {vol }}}+\underbrace{\int P_{c M} \frac{\Sigma_{a}^{U}}{\Sigma_{t}^{c}}\left(\Sigma_{t}^{c}-\Sigma_{p}^{U}\right) d u}_{I_{\text {surf }}}
$$

Thus, we obtain the notions of "volume integral" and "surface integral", discussed earlier. Using the Wigner rational approximation, $P_{c M} \approx \frac{1}{1+X} P_{c M}$ can be approached as:

$$
P_{f M} \approx \frac{1}{1+X} \quad \text { where } X \equiv \Sigma_{t}^{c}\langle R\rangle=\Sigma_{t}^{c} \frac{4 V_{c}}{S_{c}}
$$

is the opacity
This probability is valid only for an isolated object. Thus, the effective resonance integral can be simplified as:

$$
I_{e f f}^{N R}=\int \Sigma_{a}^{U}\left(\frac{\Sigma_{p}^{U}+\Sigma_{s}^{m}+\frac{4 V_{c}}{S_{c}}}{\Sigma_{t}^{U}+\Sigma_{s}^{m}+\frac{4 V_{c}}{S_{c}}}\right) d u
$$

The shadowing (Dancoff) effect must be modeled for a fuel lattice. Let us consider a simple geometry such as a lattice of fuel slabs of thickness $a$ regularly separated by a moderator of thickness $b$.


Regular lattice of slabs
For a single slab of thickness $a$, it was previously shown that the probability of leakage without collision, $P_{V S, 0}$, is equal to:

$$
P_{V S, 0}\left(\Sigma_{t}^{c} a\right)=\frac{1-\left\langle e^{-\Sigma_{t}^{c} R}\right\rangle}{\langle R\rangle}=\frac{1}{2 a \Sigma_{t}^{c}}\left[1-2 E_{3}\left(\Sigma_{t}^{c} a\right)\right] \equiv P_{V S, 0}^{a}
$$

The average value of $\left\langle e^{-\Sigma_{t}^{f} R}\right\rangle$ is proportional to the number of neutrons that are absorbed in the slab. In a slab lattice, a neutron travelling in a straight line may cross several layers of slabs and moderators before interacting far away in the moderator. Thus, probability $P_{c M}$ is modified. The slabs are numbered from left to right (cf. the illustration) starting at 0 . Hence, by combining the transfer probabilities (indexed
from the top by the slab numbers) with the probability $P_{V V}^{1 \rightarrow 1}$ of an incoming neutron in moderator volume 1 undergoing a collision in the same volume (the other probabilities are logically deduced from this notation), the following equation is obtained:

$$
\begin{aligned}
P_{c M}= & P_{c M}^{0 \rightarrow 1}+P_{c M}^{0 \rightarrow 3}+P_{c M}^{0 \rightarrow 5}+\cdots \\
= & P_{V S, 0}^{0 \rightarrow 1} P_{V V}^{1 \rightarrow 1}+P_{V S, 0}^{0 \rightarrow 1}\left(1-P_{V V}^{1 \rightarrow 1}\right) P_{V S, 0}^{2 \rightarrow 3} P_{V V}^{3 \rightarrow 3}+P_{V S, 0}^{0 \rightarrow 1}\left(1-P_{V V}^{1 \rightarrow 1}\right) P_{V S, 0}^{2 \rightarrow 3}\left(1-P_{V V}^{333}\right) \\
& P_{V S, 0}^{4 \rightarrow 5} P_{V V}^{5 \rightarrow 5}+\ldots
\end{aligned}
$$

At this point, any thickness of the fuel layers and of the moderator are considered. The problem is greatly simplified if the lattice has a constant pitch $(a, b)$ since:

$$
\left\{\begin{array}{lll}
\forall i, \forall j & P_{V S, 0}^{2 i+2 i+1}=P_{V S, 0}^{2 j \rightarrow 2 j+1} \equiv P_{V S, 0}^{a} & \text { in the fuel } \\
\forall i, \forall j & P_{V V}^{2 i+1 \rightarrow 2 i+1}=P_{V V}^{2 j+1 \rightarrow 2 j+1} \equiv P_{V V}^{b} & \text { in the moderatorr }
\end{array}\right.
$$

Hence, for an infinite lattice, the following is obtained:

$$
\begin{aligned}
P_{f M} & =P_{V S, 0}^{a} P_{V V}^{b}+P_{V S, 0}^{a}\left(1-P_{V V}^{b}\right) P_{V S, 0}^{a} P_{V V}^{b}+P_{V S, 0}^{a}\left(1-P_{V V}^{b}\right) P_{V S, 0}^{a}\left(1-P_{V V}^{b}\right) P_{V S, 0}^{a} P_{V V}^{b}+\ldots \\
& =P_{V S, 0}^{a} P_{V V}^{b}\left(1+\left(1-P_{V V}^{b}\right) P_{V S, 0}^{a}+\left(1-P_{V V}^{b}\right)^{2} P_{V S, 0}^{a}+\ldots\right) \\
& =\frac{P_{V S, 0}^{a} P_{V V}^{b}}{1-\left(1-P_{V V}^{b}\right) P_{V S, 0}^{a}}
\end{aligned}
$$

With:

$$
\begin{aligned}
P_{V S, 0}^{a} & =\frac{1}{2 a \Sigma_{t}^{c}}\left[1-2 E_{3}\left(\Sigma_{t}^{c} a\right)\right] \quad \text { and } \quad P_{V V}^{b}=1-P_{V S, 0}^{b} \\
& =1-\frac{1}{2 b \Sigma_{t}^{M}}\left[1-2 E_{3}\left(\Sigma_{t}^{M} b\right)\right]
\end{aligned}
$$

For a finite lattice, the infinite series cannot be substituted by its limit. Replacing the expression of $P_{c M}$ that accounts for the Dancoff effect in the resonance integral, it can be seen that the latter is modified with respect to the value obtained for a single slab. The foregoing idea can be summed up as follows: "a fuel cannot absorb a neutron that has been absorbed by a neighboring fuel pin". This calculation may be extended to any geometry other than a slab geometry at the expense of complex calculations for collision probabilities. This shadowing effect also exists for non-fissile absorbing materials such as control rods. Thus, the resulting absorption of two rods inserted in proximity in the core is not equal to the sum of the separate absorption of each rod.

### 14.3.7 Heterogeneous $\mathbf{P}_{\mathrm{i}, \mathrm{j}}$ Calculations for Fast Reactors with Perturbation Methods

Storrer, Khairallah, Cadilhac and Benoit developed an ingenious use of the collision probability method $P_{i, j}$ in perturbation theory. ${ }^{26,27}$ They proposed a means of calculating the effect on $k_{\text {eff }}$ of the pin-by-pin flux structure due to heterogeneity, which can be considered as a perturbation of the piecewise homogeneous case. The authors pointed out that a first-order approach based on classical perturbation theory using the spatial direct and adjoint flux for a homogeneous reactor does not induce any variation in $k_{\text {eff. }}$ However, a more appropriate formalism can be developed for the case in which the adjoint flux depends not only on the position and the energy, but also on the nature of the ensuing collision. This adjoint flux can be employed in perturbation and leads to a variation in $\delta k_{\text {eff }}$ even for a homogeneous reactor. We use the $P_{i, j}$ theory for neutrons emitted at $i$ interacting in $j$ with the flat source approximation, which is acceptable if the mean chord in each region is not too large compared to the mean free path of the neutron. In this case, a homogeneous infinite medium and a heterogeneous medium with the same mean composition are described by the same set of coupled equations between the zones, except for values of $P_{i, j}$, which change. Using the usual notations:

$$
V_{j} \Sigma_{t, j}(E) \Phi_{j}(E)=\sum_{i=1}^{n} V_{i} P_{i, j}(E) S_{i}(E)
$$

In a multi-group approach with $G$ groups and $n$ zones, we define coefficients $\overline{\bar{\Sigma}}{ }_{i}^{g^{\prime} \rightarrow g}$ such that:

$$
V_{i} S_{i}^{g}=V_{i}\left(\frac{\chi_{g} \sum_{g^{\prime}=1}^{G} v \Sigma_{f, g^{\prime}} \Phi_{i, g^{\prime}}}{k_{e f f}}+\sum_{g^{\prime}=1}^{G} \Sigma_{s, g^{\prime} \rightarrow g} \Phi_{i, g^{\prime}}\right) \equiv \underbrace{\left(\sum_{j=1}^{n} V_{j}\right)}_{V}\left(\sum_{g^{\prime}=1}^{G} \overline{\bar{\Sigma}}_{i}^{g^{\prime} \rightarrow g} \Phi_{i, g^{\prime}}\right)
$$

Thus, the equation for $P_{i, j}$ collision probabilities can be expressed in the form:

$$
\overline{\bar{\Sigma}}_{t, j, g} \Phi_{j, g}=\sum_{i=1}^{n} \sum_{g^{\prime}=1}^{G} \overline{\bar{\Sigma}}_{i}^{g^{\prime} \rightarrow g} P_{i, j}^{g^{\prime}} \Phi_{i, g^{\prime}} \quad \text { by defining } \overline{\bar{\Sigma}}_{t, j, g} \equiv \frac{V_{j}}{V} \Sigma_{t, j, g}
$$

[^299]It may be observed that the normalized cross sections $\overline{\bar{\Sigma}}$ per unit volume do not vary for a medium of given average composition, whether it is homogeneous or heterogeneous. Only the $P_{i, j}$ probabilities are impacted by heterogeneity effects. The adjoint equation is written by transposing the transport matrix:

$$
\begin{equation*}
\text { Adjoint equation: } \quad \overline{\bar{\Sigma}}_{t, j, g} \Phi_{j, g}^{*}=\sum_{i=1}^{n} \sum_{g^{\prime}=1}^{G} \overline{\bar{\Sigma}}_{j}^{g \rightarrow g^{\prime}} P_{j, i}^{g^{\prime}} \Phi_{i, g^{\prime}}^{*} \tag{14.8}
\end{equation*}
$$

Thus:

$$
\begin{equation*}
\text { Coupling of adjoint flux: } \quad \Phi_{j, g}^{*}=\sum_{i=1}^{n} \sum_{g^{\prime}=1}^{G} \frac{\overline{\bar{\Sigma}}_{j}^{g \rightarrow g^{\prime}}}{\overline{\bar{\Sigma}}_{t, j, g}} P_{j, i}^{g^{\prime}} \Phi_{i, g^{\prime}}^{*} \tag{14.9}
\end{equation*}
$$

Ratio $\overline{\bar{\Sigma}}_{j}^{g \rightarrow g^{\prime}} / \overline{\bar{\Sigma}}_{t, j, g}$ is the probability of a neutron emitted in group $g$ in the region $j$ leading to a neutron in group $g^{\prime}$ in the same region. $P_{j, i}^{g^{\prime}}$ is the probability that the same neutron produced will undergo a collision in the next zone $i$ and thus $\Phi_{j, g}^{*}$ is the contribution of a neutron in group $g$ undergoing its next collision in zone $j$. This definition differs from neutron importance as discussed in the chapter on the transport equation. If applied to the particular case of a homogeneous medium, the probability $P_{i, j}^{g}$ is that of a neutron in group $g$ which last collided in region $i$ undergoing its next collision in zone $j$. This probability does not depend on $i$ due to the homogeneity hypothesis:

$$
P_{i, j \text { Homog }}^{g}=\frac{\overline{\bar{\Sigma}}_{t, j, g}}{\overline{\bar{\Sigma}}_{t, g}}=\frac{\overline{\bar{\Sigma}}_{t, j, g}}{\Sigma_{t, g}} \quad \text { since: } \quad \overline{\bar{\Sigma}}_{t, g} \equiv \sum_{j=1}^{n} \overline{\bar{\Sigma}}_{t, j, g}=\Sigma_{t, g}
$$

With these homogeneous probabilities $P_{i, j}$, flux $\Phi_{j, g}$ does not depend on zone $j$ and satisfies the usual homogeneous equation:

$$
\overline{\bar{\Sigma}}_{t, g} \Phi_{g}=\sum_{g^{\prime}=1}^{G} \overline{\bar{\Sigma}}^{g^{\prime} \rightarrow g} \Phi_{g^{\prime}} \quad \text { with: } \quad \overline{\bar{\Sigma}}^{g^{\prime} \rightarrow g}=\sum_{i=1}^{n} \overline{\bar{\Sigma}}_{i}^{g^{\prime} \rightarrow g}
$$

Nevertheless, the homogeneous adjoint equation is not simply the neutron importance equation $I_{g}$ given by:

$$
\overline{\bar{\Sigma}}_{t, g} I_{g}=\sum_{g^{\prime}=1}^{G} \overline{\bar{\Sigma}}^{g \rightarrow g^{\prime}} I_{g^{\prime}}
$$

Substituting $P_{j, i}^{g^{\prime}}$ by its value for the homogeneous case $P_{j, i}^{g_{H o m o g}}$ in Eq. (14.9), and dividing each side by $\overline{\bar{\Sigma}}_{t, g}$, the following equation is obtained:

$$
\Phi_{j, g_{\text {Homog }}}^{*}=\sum_{g^{\prime}=1}^{G} \frac{\overline{\bar{\Sigma}}_{j}^{g \rightarrow g^{\prime}}}{\overline{\bar{\Sigma}}_{t, j, g}} I_{g^{\prime}}
$$

Therefore, $\Phi_{j, g_{\text {Homog }}}^{*}$ depends on $j$ even for a homogeneous situation, unlike neutron importance, which is the adjoint flux corresponding to a particular boundary condition as discussed earlier. Using the operators introduced in the paragraph on the perturbation approach in Chap. 11, the transport equation is expressed as:

$$
(K-\lambda P)[\Phi]=0
$$

where $K\left[\right.$ ] is the removal operator and $P\left[\right.$ ] is the production operator, with $\lambda \equiv 1 / k_{\text {eff }}$ being the eigenvalue. In Chap. 11, it was shown that the first-order perturbation is written as:

$$
\frac{\delta k_{e f f}}{k_{\text {eff }}}=-\frac{\delta \lambda}{\lambda}=-\frac{\left\langle\Phi^{*},(\delta K-\lambda \delta P)[\Phi]\right\rangle}{\lambda\left\langle\Phi^{*}, K[\Phi]\right\rangle}
$$

In multi-group and multi-cell approximation, the transport operator is a $n \times G$ matrix in which the coefficients are linear combinations of the $P_{i, j}$, which depend on heterogeneity, unlike the normalized cross sections. A perturbation $\delta P_{i, j}^{g} \equiv P_{i, j_{\text {Heetrog }}}^{g}-P_{i, j_{\text {Homog }}}^{g}$ due to heterogeneity originating in a non-perturbed situation leads to the first-order perturbation of $\delta k_{\text {eff }}$ such that (all coefficients have been calculated):

$$
\frac{\delta k_{e f f}}{k_{e f f}}=\sum_{g=1}^{G} \frac{\sum_{j=1}^{n} \Phi_{j, g_{\text {Homog }}}^{*} \sum_{i=1}^{n} \delta P_{i, j}^{g} \sum_{g^{\prime}=1}^{G} \overline{\bar{\sum}}^{g^{\prime} \rightarrow g} \Phi_{i, g_{H o m o g}^{\prime}}}{\sum_{g^{\prime}=1}^{G} \sum_{j=1}^{n} \Phi_{j, g_{\text {Homog }}^{\prime}} \sum_{i=1}^{n} P_{i, j_{\text {Homog }}}^{g^{\prime}} \chi_{g^{\prime}} \sum_{g^{\prime \prime}=1}^{G} v \overline{\bar{\sum}}_{f, i, g^{\prime \prime}} \Phi_{i, g_{H o m o g}^{\prime \prime}}}
$$

With the expressions of $P_{i, j_{\text {Homog }}}^{g^{\prime}}, \Phi_{i, g_{\text {Homog }}^{\prime}}$ and $\Phi_{j, g_{\text {Homog }}}^{*}$, determined earlier, the following equation is reached:

$$
\frac{\delta k_{e f f}}{k_{e f f}}=\sum_{g=1}^{G} \frac{\sum_{j=1}^{n}\left[\sum_{g^{\prime}=1}^{G} \frac{\overline{\bar{\Sigma}}_{j}^{g \rightarrow g^{\prime}}}{\overline{\bar{\Sigma}}_{t, j}^{g}} I_{g^{\prime}} \sum_{i=1}^{n} \delta P_{i, j}^{g} \sum_{g^{\prime \prime}=1}^{G} \overline{\bar{\Sigma}}_{i}^{g^{\prime \prime} \rightarrow g} \Phi_{g^{\prime \prime}}\right]}{\left(\sum_{g^{\prime}=1}^{G} \chi_{g^{\prime}} I_{g^{\prime}}\right)\left(\sum_{g^{\prime \prime}=1}^{G} v \overline{\bar{\Sigma}}_{f, g^{\prime \prime}} \Phi_{g^{\prime \prime}}\right)} \text { with }: \overline{\bar{\Sigma}}_{f, g^{\prime \prime}} \equiv \sum_{i=1}^{n} \overline{\bar{\Sigma}}_{f, i, g^{\prime \prime}}
$$

With $G$ adjoint calculations, with perturbation in the group $g$ and without perturbation in the other groups, $G$ flux maps are obtained, leading to $G$ values of $\left(\delta k_{\text {eff }} / k_{\text {eff }}\right)_{g}$. Global perturbation is calculated by summing all these contributions as follows:

$$
\frac{\delta k_{e f f}}{k_{\text {eff }}}=\sum_{g=1}^{G}\left(\frac{\delta k_{\text {eff }}}{k_{\text {eff }}}\right)_{g}
$$

The flux variation can be evaluated from the variation in the eigenvalue. This method has been successfully used to calculate the Doppler effect due to a heterogeneous temperature variation with respect to a homogeneous reference situation. Furthermore, it illustrates the use of perturbations for parametric studies since their calculation is fairly expensive, along with $G+1$ homogeneous calculations to be carried out ( 1 homogeneous direct calculation and $G$ homogeneous adjoint ones). The computation cost is low, especially when compared to the direct heterogeneous case. Nevertheless, progress in computational power means that direct heterogeneous calculations are preferred to those with perturbations. Nevertheless, this method enables evaluation of the differential coefficients for the perturbation considered. These coefficients are essential for simplified models and for understanding complex physical phenomena.

### 14.4 Transport-Diffusion Equivalence

(Homogenization methods in reactor physics 1980; Reuss 2003, p. 390)

### 14.4.1 Context

Calculation of a reactor in 3D continues to be very challenging in exact transport theory. For industrial purposes, reactors are calculated using a simplified method, which in most cases is the diffusion approximation. In this context, the reactor is calculated in two steps. First, a transport calculation ${ }^{28}$ is carried out on a reference pattern representative of the periodicity of the reactor lattice, and with sufficient precision to represent the local physics (guide thimble, void regions, highly absorbing materials, etc.): this is called an elementary calculation, a cell calculation or a basic cell lattice. This calculation is often called a heterogeneous calculation or assembly calculation, since the fuel assembly is often the elementary cell of the core. It is usually carried out with reflective boundary conditions to represent an

[^300]

Fig. 14.17 Step 1: Transport calculation and homogenization (example of a PWR assembly)
infinite lattice. In thermal neutron reactors, the mean free path of neutrons is of the same order of magnitude as the lattice heterogeneity. Thus, the flux, especially the thermal flux, undergoes high spatial distortions due to variation in the spectral index. Therefore, the heterogeneous geometry cannot easily be homogenized as a homogeneous medium (Fig. 14.17) compatible with the homogeneous simplified solver. The simplest homogenization ${ }^{29}$ consists in weighting the macroscopic cross sections by the volumes and the flux calculated in transport theory so as to conserve the reaction rates used universally as physical quantities in the neutron balance.

Next, using homogenized neutron properties from the previous step, a coarser calculation is carried out at the core level. The latter is the core calculation in which each assembly is modeled as a homogeneous material per thermal-hydraulic mesh cell. Using the neutron quantities obtained from homogenized transport calculations without any particular correction in the diffusion calculation at the core level leads to reaction rates that differ between heterogeneous transport and homogeneous diffusion. This discrepancy is caused by several factors: differences in solver and meshes, and thus in leakage. These calculations can be improved by the transport-diffusion equivalence. ${ }^{30}$ It may be noted that at the homogenized assembly level in an infinite lattice, the homogeneous diffusion equation and the homogeneous transport equation can be summed up as a neutron balance without leakage (the leakage current being zero at the boundary thanks to the "infinite medium" calculation). This means that homogeneous diffusion calculations driven by cross sections obtained through the homogeneous transport calculations under the same conditions-which will be called transport cross sections-will lead to the same reference reaction rates as for the homogeneous transport method. Thus, transport cross sections can be used as such in diffusion calculations. Equivalence, i.e. the operation consisting in modifying transport cross sections via an equivalence

[^301]coefficient such that the diffusion calculation is equivalent to the transport calculation, is unnecessary in an infinite lattice. The neutron balance and $k_{\text {eff }}$ are conserved by construction. Nevertheless, the fluxes at the interfaces are not generally conserved. Further, spectrum variations at the interfaces are not considered since transport calculations are carried out in an infinite lattice approximation. In practice, an assembly is often surrounded by different assemblies rather than identical ones, which means that, in the case of an infinite lattice there is no need for equivalence. This textbook case does not have any practical applications. Usually, the assembly is calculated in heterogeneous transport theory with a fine mesh, whereas that of diffusion is coarser (of the order of a few cm). Diffusion theory will thus predict reaction rates that differ from the transport method if the cross sections from a transport calculation are used immediately in calculations (especially near sources and interfaces). In order to ensure equivalence between the initial heterogeneous transport and diffusion, trans-operator equivalence, usually transport-diffusion, should be carried out (although transport-transport equivalence is possible between a collision probability operator $P_{i j}$ and an $S_{n}$ method). Equivalence between a heterogeneous diffusion solver with a fine mesh and the same solver with a coarser mesh may even be considered; in this case, equivalence would catch up with the mesh effect rather than the operator effect.

### 14.4.2 Spatial Homogenization

The ideal homogenization process would conserve all the reaction rates with respect to the reference situation (fine transport) at any point in space. Let $\widehat{\Phi}$ and $\widehat{\Sigma}$ be the homogenized quantities. The quantity to conserve is:

$$
\int_{V} \widehat{\Sigma}(\vec{r}) \widehat{\Phi}(\vec{r}) d \vec{r}=\int_{V} \Sigma(\vec{r}) \Phi(\vec{r}) d \vec{r}
$$

Thus, the evident definition for homogenized neutron quantities on a cell is:

$$
\widehat{\Sigma}=\frac{\int_{V} \Sigma(\vec{r}) \Phi(\vec{r}) d \vec{r}}{\int_{V} \widehat{\Phi}(\vec{r}) d \vec{r}}
$$

the homogenized diffusion coefficient satisfies the following equation to preserve the total leakage of the cell:

$$
\widehat{D}=-\frac{\int_{S} \vec{J}(\vec{r}) \cdot \vec{n} d S}{\int_{V} \overrightarrow{g r a d} \widehat{\Phi}(\vec{r}) \cdot \vec{n} d S}
$$

These equations show the difficulty of the homogenization process. The weighting flux for homogenizing physical quantities is the spatial flux of the homogenized calculation itself, $\widehat{\Phi}$, which is the quantity being sought. Hence, the result is a non-linear problem that should be dealt with using an iterative process since the flux solution is not known in advance. On the other hand, exact homogenization of the diffusion coefficient includes the cell surface. In practical cases, only a reference flux obtained with transport calculations on an infinite lattice geometry is available (denoted as $\Phi_{\infty}(\vec{r})$ for each spatial zone to be homogenized, usually an assembly). This flux is used to homogenize the neutron quantities:

$$
\widehat{\Sigma}=\frac{\int_{V} \Sigma(\vec{r}) \Phi_{\infty}(\vec{r}) d \vec{r}}{\int_{V} \Phi_{\infty}(\vec{r}) d \vec{r}} \text { and } \widehat{D}=\frac{\int_{V} D(\vec{r}) \Phi_{\infty}(\vec{r}) d \vec{r}}{\int_{V} \Phi_{\infty}(\vec{r}) d \vec{r}}
$$

However, by definition, the flux in an infinite lattice cannot account for leakage. Several codes employ a countermeasure that consists in adding a fictitious isotope having the properties to account for leakage:

- Either by imposing an absorption cross section $\Sigma_{a}=D B^{2}$ and scattering cross section $\Sigma_{s}=-D B^{2}$, such that the total cross section is zero, with $D$ and $B^{2}$ being the diffusion coefficient and the buckling of the homogeneous medium.
- Or by setting only an absorption cross section worth $\Sigma_{a}=D B^{2}$ and a zero scattering cross section.
The following steps are carried out: a first calculation is carried out and consists in homogenizing the cell media by weighting with a heterogeneous flux from the infinite lattice (zero leakage). Then, using a transport calculation (with the $B_{n}$ or $P_{n}$ method discussed in Chap. 9), $D$ and $B^{2}$, i.e. the properties of the fictitious isotope, are calculated. This iterative process is repeated until convergence to the chosen $k_{\text {eff }}$ (1 for a critical geometry).


### 14.4.3 Multi-group Approach

In most industrial cases, calculations are carried out with few energy groups (often two groups are sufficient), and with a simple method (diffusion, simplified transport). The conservation of multi-group reaction rates is carried out iteratively. The goal is to conserve the reaction rate for a given reaction cross section $\kappa$ (total, fission, etc.) in diffusion $\Sigma_{\kappa, \text { diffusion }}^{g} \Phi_{\text {diffusion }}^{g}$ with respect to a transport value $\Sigma_{\kappa, \text { transport }}^{g} \Phi_{\text {transport }}^{g}$ for each group $g$. The simplest solution is to modify the diffusion cross sections using an equivalence coefficient per calculation cell, $\mu^{g}$, that is unique for all reaction cross sections but different for each energy group. If a one-energy
group diffusion calculation were carried out, modification of all the cross sections with a multiplication factor would not change the flux solution, but this is no longer the case in multi-group theory if the equivalence coefficients are different in each group. The equivalence process consists of an iterative calculation in which cross sections are modified until the reaction rates are equal for both the transport and diffusion calculations. In our approach, if all equivalence coefficients are constant for any reaction (but different for each energy group), the chosen reaction rate to be conserved does not matter. Indeed, the conservation of one reaction rate ensures that of the others:
$\Sigma_{t, \text { diffusion }}^{g} \Phi_{\text {diffusion }}^{g}=\Sigma_{t, \text { transport }}^{g} \Phi_{\text {transport }}^{g} \Rightarrow \Sigma_{\kappa, \text { transport }}^{g}\left(\mu^{g} \Sigma_{t, \text { transport }}^{g}\right) \Phi_{\text {diffusion }}^{g}$
$=\Sigma_{\kappa, \text { transport }}^{g} \Sigma_{t, \text { transport }}^{g} \Phi_{\text {transport }}^{g}$

Thus: $\left(\mu^{g} \Sigma_{\kappa, \text { transport }}^{g}\right) \Phi_{\text {diffusion }}^{g}=\Sigma_{\kappa, \quad \text { transport }}^{g} \Phi_{\text {transport }}^{g} \Rightarrow \Sigma_{\kappa, \text { diffusion }}^{g} \Phi_{\text {diffusion }}^{g}$ $=\sum_{\kappa, \text { transport }}^{g} \Phi_{\text {transport }}^{g}$

Finally, whether for a transport or diffusion operator, it can be noted that if $\Phi^{g}$ were the solution to the problem for cross sections $\Sigma_{k}^{g}$, then $\Phi^{g} / \mu^{g}$ would be a solution to the same problem for cross sections $\mu^{g} \sum_{\kappa}^{g}$. This implies that the equivalence coefficients are defined up to a multiplication constant for each energy group. Using a closure property, the equivalence coefficient can be normalized and fully defined. For instance, we can use the flux integrated in space (for all the cells $m$ of volumes $V_{m}$ ) per group:

$$
\sum_{m} V_{m} \Phi_{\text {diffusion }, m}^{g}=\sum_{m} V_{m} \Phi_{\text {transport }}^{g} \Rightarrow \sum_{m} \frac{V_{m}}{\mu^{g}}=\sum_{m} V_{m}
$$

The equivalence coefficients could also be normalized to the power dissipated per energy group or other considerations, which will be discussed later.

### 14.4.4 Kavenoky-Hébert SPH Equivalence

(Hébert 2009, p. 247)
The SPH (SuPerHomogenization) equivalence initially proposed by Alain Kavenoky ${ }^{31}$ in 1978, subsequently developed and improved by Alain

[^302]Hébert, ${ }^{32,33,34}$ is an extension of the previous method applied to any geometry of macro-cells. A macro-cell is a group of cells, $m$, in the fine transport calculation from a geometrical point of view as well as the number of groups. Its volume is the sum of cell volumes of which it consists:

$$
V_{M}=\sum_{m \in M} V_{m}
$$

Similarly, for a macro-group $G$ in energy, there will be several fine groups $g$. The number of collisions in transport in a macro-group and a macro-cell is given by a simple flux-volume homogenization:

$$
R_{M, G}=\sum_{m \in M} \sum_{g \in G} V_{m} \Sigma_{t, m, g} \Phi_{m, g}
$$

The leakage ( $L$ ) and self-scattering terms (S) are given by ${ }^{35}$ :

$$
\left\{\begin{array}{l}
L_{M, G}=B^{2} \sum_{g \in G} D_{g} \sum_{m \in M} V_{m} \Phi_{m, g} \\
S_{M, G \rightarrow G}=\sum_{m \in M} \sum_{g \in G} \sum_{g^{\prime} \in G} V_{m} \Sigma_{s, m, g^{\prime} \rightarrow g} \Phi_{m, g^{\prime}}-B^{2} \sum_{g \in G} D_{g} \sum_{m \in M} V_{m} \Phi_{m, g}
\end{array}\right.
$$

Fission production $(P)$ and slowing down from other macro-groups are given by:

$$
\begin{aligned}
P_{M, G^{\prime} \rightarrow G}= & \sum_{m \in M} \sum_{g \in G} \sum_{g^{\prime} \in G^{\prime}} V_{m} \Sigma_{s, m, g^{\prime} \rightarrow g} \Phi_{m, g^{\prime}}+\sum_{m \in M} \sum_{g \in G} \sum_{g^{\prime} \in G^{\prime}} V_{m} \chi_{g} \frac{v \Sigma_{f, m, g^{\prime}} \Phi_{m, g^{\prime}}}{k_{e f f}} \\
& -\delta_{G^{\prime}, G} \sum_{m \in M} \sum_{g \in G} \sum_{g^{\prime} \in G^{\prime}} V_{m} \Sigma_{s, m, g^{\prime} \rightarrow g} \Phi_{m, g^{\prime}}
\end{aligned}
$$

[^303]The integrated transport flux is expressed as:

$$
\Phi_{M, G}=\sum_{g \in G} \sum_{m \in M} V_{m} \Phi_{m, g}
$$

The transport cross sections are calculated from volume-integrated reaction rates and are used to determine diffusion cross sections through the use of equivalence coefficients for individual macro-cells and macro-groups:

$$
\left\{\begin{array}{c}
\Sigma_{t, M, G}^{\text {transport }}=\frac{R_{M, G}}{\Phi_{M, G}} \\
\Sigma_{s, M, G \rightarrow G}^{\text {transort }}=\frac{S_{M, G \rightarrow G}}{\Phi_{M, G}} \quad\left\{\begin{array}{c}
\Sigma_{t, M, G}^{\text {diffusion }}=\mu_{M, G} \Sigma_{t, M, G}^{\text {transport }} \\
\Sigma_{s, M, G \rightarrow G}^{\text {diffusion }}=\mu_{M, G} \Sigma_{s, M, G \rightarrow G}^{\text {transport }} \\
D_{M, G}^{\text {transport }}= \\
D_{M, G}^{\text {difusion }}=\mu_{M, G} D_{M, G}^{\text {transport }}
\end{array} L^{2} \Phi_{M, G}\right.
\end{array}\right.
$$

The homogenized diffusion flux that conserves a homogeneous diffusion equation is defined as:

$$
\Phi_{M, G}^{\text {diffusion }}=\frac{\Phi_{M, G}^{\text {transport }}}{\mu_{M, G}}
$$

The diffusion equation is expressed as follows with the above definitions, by dropping the dependence in $M$, which becomes the space variable:
$-\operatorname{div}\left(D_{G}^{\text {diffusion }} \overrightarrow{\operatorname{grad}} \Phi_{G}^{\text {diffuson }}\right)+\left(\Sigma_{t, G}^{\text {diffusion }}-\Sigma_{s, G \rightarrow G}^{\text {diffusion }}\right) \Phi_{G}^{\text {diffuson }}=\sum_{G^{\prime}} \frac{P_{G^{\prime} \rightarrow G} \Phi_{G^{\prime}}^{\text {difuson }}}{\frac{\Phi_{G^{\prime}}^{\text {ranport }}}{\mu_{G^{\prime}}}}$
An iterative procedure as shown in Fig. 14.18 can be set up for $\mu_{M, G}$ so as to determine the diffusion flux that satisfies the integrated transport reaction rates on the macro-cells. This reasoning can easily be extended to a case of transporttransport equivalence.

### 14.4.5 Flux Reconstruction Between Different Operators

A second ambiguous point is that the position of the hottest pin in the core is required for safety considerations, i.e. the position at which maximum power occurs (Silvennoinen 1976, p. 66). In a homogeneous core, this point is naturally at the center of the reactor. However, the materials constituting the fuel are not homogeneous in terms of isotopic composition and thermal-hydraulic parameters, and this point thus shifts within the core depending on the loading pattern and operating


Fig. 14.18 Equivalence procedure for reaction rates
conditions. Further, it is clear that this position is sought at the fuel pin level whereas the diffusion calculation is executed for a homogeneous assembly and leads to any spatial position $(x, y, z)$ that may not coincide with an actual fuel pin. Thus, the process of pin power reconstruction is required. This consists in factorizing the homogeneous power that will be wisely distributed on the true assembly lattice. Finally, it should be noted that diffusion calculations are carried
out with very few energy groups (around two to six) and thus, require energy condensations of transport calculations that are usually performed for over 200 groups. As the reactor is smaller, the boundary conditions set by the reflector will have a significant effect on the neutron spectrum which diverges from that of an infinite lattice assembly. In these cases, increasing the number of groups will lead to improved calculations. This reasoning is limited by the fact that fine energy discretization with many groups is not consistent with diffusion approximation. It is interesting to note that this two-step approach is widely employed worldwide where two-group calculations have become a standard for $P W R$ and six-energy groups for $B W R$. In the early 2000s, efforts were made to calculate small and large experimental reactors using a one-step approach with fixed conditions. The major limitation is the calculation time rather than any theoretical difficulties (Fig. 14.19).

Nevertheless, there still remains the question of how to provide the diffusion approximation with appropriate cross sections in order to obtain the transport results for quantities such as reaction rates, which are the principal quantities to be conserved. Historically, two effects are distinguished:

- the heterogeneity effect, which appears when a lattice of cells is replaced by a homogeneous medium
- the non-consistency effect, which is due to the fact that homogenized neutron quantities inserted as such in diffusion calculations lead to discrepancies with respect to transport results, especially at interfaces between media.

In France in 1959, Pierre Benoist of the CEA published in his PhD thesis a method allowing for cavity effects on the diffusion coefficient for $U N G G$. His idea was based on factorization of the flux into a macroscopic flux and a microscopic flux structure of the same spatial period as the lattice. This approach consists in writing the flux in the following form with a source expressed as:


Fig. 14.19 Step 2: Diffusion calculation (e.g. $P W R$ core)

$$
\Phi(\vec{r}, E, \vec{\Omega})=\varphi(\vec{r}, E, \vec{\Omega}) e^{-i \vec{B} \cdot \vec{r}}
$$

where $s(\vec{r}, E)$ and $\varphi(\vec{r}, E, \vec{\Omega})$ are periodic functions on the lattice and $e^{-i \vec{B} . \vec{r}}$ is the macroscopic flux. This technique, discussed in detail in Chap. 9, is equivalent to applying the Fourier transform to the flux. The diffusion coefficient can be computed from the leakage and the buckling. ${ }^{36}$

### 14.4.5.1 Reflected Medium (Infinite)

In this case, the heterogeneous and regular lattice can be substituted by a homogenized lattice which is applied infinitely. This formalism is called the homogeneous $B$ formalism (with the model being $B_{0}$ if scattering is modeled isotropically and $B_{1}$ in the case of linearly anisotropic scattering). In this situation, we therefore perform factorization with an exponential function and a microscopic function dependent solely on angle and energy, but no longer space. This factorization is possible for a unique value of the buckling term $B^{2}$, and corresponds to the critical situation with a fundamental mode flux. This homogenization theory is sometimes called the smallbuckling approximation. ${ }^{37}$ It is possible to factorize the flux only by choosing a macroscopic flux with an exponential form since its gradient is proportional to itself. The macroscopic flux satisfies a diffusion equation and the global flux is perturbed locally by the microscopic structure. The leakage is expanded into a Taylor series with respect to the buckling term and only the significant terms are considered (hence the fact that precision depends on a small degree of buckling). Hence, Benoist's theory conserves the leakage in the considered lattice cell and corrects heterogeneity and anisotropy in the diffusion calculation using the fictitious isotope method broached earlier. Thus to represent a heterogeneous critical assembly, a fictitious absorption term due to the macroscopic flux is taken into account through use of the leakage coefficient and the critical buckling obtained from the homogenized equivalent medium. This leakage coefficient and critical buckling are calculated using cross sections homogenized with the local heterogeneous flux, such that the homogeneous medium is representative of the heterogeneous medium. Since the heterogeneous flux itself depends on the leakage, this is an iterative procedure. The calculation is carried out in two steps. First, the equivalent homogeneous medium is calculated using cross sections weighted by a multi-group heterogeneous flux for the infinite (reflective boundary conditions) heterogeneous

[^304]assembly (infinite lattice). This medium cannot in theory be critical (this may be the case for nominal depletion with constant boron: the assembly is over-multiplying at $B O L$ and becomes under-multiplying at $E O L$. There consequently exists a burn-up for which the assembly will be just critical, although this is a textbook case where buckling is zero at any point). In the general case, a macroscopic leakage cross section $D_{g} B_{g}^{2}$ is considered for the homogeneous assembly for each energy group in order for it to be critical. This homogeneous critical buckling is not equal to the fundamental buckling of the heterogeneous assembly since the cross sections are those homogenized by a heterogeneous infinite-lattice flux not taking account of leakage. A second calculation is hence carried out for the reflected heterogeneous assembly with a further volume-wise absorption term, in addition to the absorption cross section $D_{g} B_{g}^{2}$ evaluated from the previous homogeneous calculation. This is referred to as "volume leakage." The iteration proceeds on until criticality is reached for the heterogeneous assembly. The drawback of this method is the fact that leakage is calculated for the homogeneous assembly and not the real heterogeneous assembly. This implies that the leakage cross section $D_{g} B_{g}^{2}$ should rigorously depend on space, which is not the case for homogeneous leakage through construction. Furthermore, the anisotropy of the medium (for instance, cavities that lead to a streaming effect) is not correctly allowed for by the method, which only caters for this effect through the volume weighting of cross sections. Further, there is also the flux factorization hypothesis, which assumes that there is only the fundamental mode, which may not be the case since higher harmonics may exist due to the interfaces. ${ }^{38}$

### 14.4.5.1.1 Homogeneous $B_{0}$ Model

(Hébert 2005, p. 232)
Let us start from the multi-group integro-differential equation with an isotropic scattering hypothesis and constant cross sections due to the infinite homogeneous medium:

[^305]\[

$$
\begin{aligned}
& \vec{\Omega} \cdot \overrightarrow{g r a d} \Phi_{g}(\vec{r}, \vec{\Omega})+\Sigma_{t}^{g} \Phi_{g}(\vec{r}, \vec{\Omega}) \\
& \quad=\frac{1}{4 \pi}\left(\sum_{g^{\prime}} \Sigma_{s, 0}^{g^{\prime} \rightarrow g} \int_{4 \pi} \Phi_{g^{\prime}}(\vec{r}, \vec{\Omega}) d \vec{\Omega}+\chi_{g} \sum_{g^{\prime}} \frac{v \Sigma_{f}^{g^{\prime}} \int_{4 \pi} \Phi_{g^{\prime}}(\vec{r}, \vec{\Omega}) d \vec{\Omega}}{k_{e f f}}\right)
\end{aligned}
$$
\]

The notations are simplified by:

$$
\Sigma_{0}^{g^{\prime} \rightarrow g} \equiv \Sigma_{s, 0}^{g^{\prime} \rightarrow g}+\chi_{g} v \Sigma_{f}^{g^{\prime}}
$$

The following energy-space flux factorization is inserted for each group:

$$
\Phi_{g}(\vec{r}, \vec{\Omega})=\varphi_{g}(\vec{r}, \vec{\Omega}) e^{-i \vec{B} \cdot \vec{r}}
$$

For a critical medium $\left(k_{e f f}=1\right)$ :

$$
\left(i \vec{B} . \vec{\Omega}+\Sigma_{t}^{g}\right) \varphi_{g}(\vec{\Omega})=\frac{1}{4 \pi}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \int_{4 \pi} \varphi_{g^{\prime}}(\vec{\Omega}) d \vec{\Omega}\right)
$$

Integrating over the unit sphere ( $4 \pi$ steradians), we obtain:

$$
\begin{align*}
\varphi_{g} \equiv \int_{4 \pi} \varphi_{g}(\vec{\Omega}) d \vec{\Omega} & =\int_{4 \pi} d \vec{\Omega} \frac{1}{4 \pi\left(i \vec{B} \cdot \vec{\Omega}+\Sigma_{t}^{g}\right)}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \int_{4 \pi} \varphi_{g^{\prime}}(\vec{\Omega}) d \vec{\Omega}\right) \\
& =\frac{1}{4 \pi} \int_{0}^{2 \pi} d \varphi \int_{0}^{\pi} \frac{\sin \theta d \theta}{\Sigma_{t}^{g}+i B \cos \theta}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}\right) \\
& =\frac{1}{2 \pi} \int_{-1}^{+1} \frac{d \mu}{\Sigma_{t}^{g}+i B \mu}\left(\sum_{g^{\prime}} \Sigma_{O}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}\right) \\
& =\frac{1}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}\right) \tag{14.10}
\end{align*}
$$

It may be noted that the same buckling is used for all the groups. The smallest real value of $B^{2}$ is the critical buckling for the medium.

The current is expressed as:

$$
\begin{aligned}
\vec{J}_{g}(\vec{r}) & \equiv \int_{4 \pi} \vec{\Omega} \Phi_{g}(\vec{r}, \vec{\Omega}) d \vec{\Omega}=e^{i \vec{B} \vec{r}} \int_{4 \pi} \vec{\Omega} \varphi_{g}(\vec{\Omega}) d \vec{\Omega} \\
& =e^{i \vec{B} \vec{r}} \sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}} \int_{4 \pi} \vec{\Omega} d \vec{\Omega} \frac{1}{4 \pi\left(i \vec{B} \cdot \vec{\Omega}+\Sigma_{t}^{g}\right)}
\end{aligned}
$$

In Chap. 9, this type of integral was introduced, setting $\vec{B}=B \vec{z}$ along the $z$ axis such that the $\vec{x}$ and $\vec{y}$ terms are zero. Thus:

$$
\begin{aligned}
\int_{4 \pi} \vec{\Omega} d \vec{\Omega} \frac{1}{4 \pi\left(i \vec{B} \cdot \vec{\Omega}+\Sigma_{t}^{g}\right)} & =2 \pi \int_{-1}^{+1} \frac{\mu d \mu}{\Sigma_{t}^{g}+i B \mu} \vec{z}=\frac{2 \pi}{i B} \int_{-1}^{+1} \frac{B^{2} \mu^{2} d \mu}{\Sigma_{t}^{g} 2+B^{2} \mu^{2}} \vec{z} \\
& =\frac{4 \pi}{i B^{2}}\left(1-\frac{\Sigma_{t}^{g}}{B} \tan ^{-1} \frac{B}{\Sigma_{t}^{g}}\right) \vec{B}
\end{aligned}
$$

$\vec{J}_{g}(\vec{r})$ is colinear to $\vec{B}$. If $\vec{B}$ had been chosen in any other direction, the same result would have been reached, i.e.:

$$
\left\{\begin{array}{l}
\vec{J}_{g}(\vec{r}) \equiv e^{i \vec{B} \vec{r}} \vec{j}_{g}=e^{i \vec{B} \vec{r}} \sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}} \frac{1}{i B^{2}}\left(1-\frac{\Sigma_{t}^{g}}{B} \arctan \frac{B}{\sum_{t}^{g}}\right) \vec{B}=-D_{g} g \overrightarrow{r a} d \Phi_{g}(\vec{r}) \\
\vec{j}_{g}=-i D_{g} \vec{B} \varphi_{g}
\end{array}\right.
$$

This equation is obtained by substituting $\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}$ by $\varphi_{g} B / \arctan \frac{B}{\Sigma_{t}^{8}}$, as given by Eq. (14.10) and the group-wise diffusion term is defined as:

$$
D_{g} \equiv \frac{1}{B} \frac{\left(1-\frac{\Sigma_{t}^{g}}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\right)}{\arctan \frac{B}{\Sigma_{t}^{g}}}=\frac{1}{3 \Sigma_{t}^{g}}\left(1-\frac{4}{15} \frac{B^{2}}{\Sigma_{t}^{g^{2}}}+O\left(\frac{B^{4}}{\Sigma_{t}^{g^{4}}}\right)\right)
$$

The analogy with Fick's law in diffusion should be noted. In an infinite homogeneous medium, the only hypothesis employed is isotropic scattering, thereby showing the asymptotic behavior of transport theory far from boundaries. The "usual" diffusion coefficient $D=1 /\left(3 \Sigma_{t}\right)$ is the limit of the coefficient $D_{g}$ when the buckling of the system tends towards 0 . If the system is over-critical, the buckling term is real, whereas for subcritical cases, it is purely imaginary, i.e. $B=i|B|$ and $B^{2}=-|B|^{2}<0$. In this case, the following equation which was illustrated earlier is used:

$$
\arctan \frac{i B}{\Sigma_{t}^{g}}=\frac{i}{2} \ln \frac{\Sigma_{t}^{g}+B}{\Sigma_{t}^{g}-B} \quad \text { Hence: } \quad D_{g} \equiv-\frac{1}{B} \frac{\left(1-\frac{\Sigma_{t}^{g}}{2 B} \ln \frac{\Sigma_{t}^{g}+B}{\Sigma_{t}^{g}-B}\right)}{\frac{1}{2} \ln \frac{\Sigma_{t}^{g}+B}{\Sigma_{t}^{g}-B}}
$$

It can be seen that the diffusion coefficient of group $g$ depends solely on the total cross section of the same group. Due to the isotropic scattering hypothesis, there is no coupling with other energy groups.

### 14.4.5.1.2 Homogeneous $B_{1}$ Model

In the homogeneous $B_{1}$ model, the scattering cross section is expanded to order 1, i.e.:

$$
\Sigma_{s}^{g^{\prime} \rightarrow g}\left(\vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)=\frac{1}{4 \pi}\left(\sum_{s, 0}^{g^{\prime} \rightarrow g}+\sum_{s, 1}^{g^{\prime} \rightarrow g} \vec{\Omega} \cdot \vec{\Omega}^{\prime}\right)
$$

This expression is inserted in the Boltzmann equation, and by similar calculations as for the homogeneous $B_{0}$ model, with an additional term as $\vec{\Omega} \cdot \vec{\Omega}^{\prime}$, the following equation is reached:

$$
\left\{\begin{array}{l}
\left(i \vec{B} \cdot \vec{\Omega}+\Sigma_{t}^{g}\right) \varphi_{g}(\vec{\Omega})=\frac{1}{4 \pi}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \int_{4 \pi} \varphi_{g^{\prime}}(\vec{\Omega}) d \vec{\Omega}+\sum_{s, 1}^{g^{\prime} \rightarrow g} \vec{\Omega} \cdot \overrightarrow{j_{g^{\prime}}}\right)  \tag{14.11}\\
\vec{j}_{g^{\prime}} \equiv \int_{4 \pi} \Phi_{g^{\prime}}\left(\vec{\Omega}^{\prime}\right) \vec{\Omega}^{\prime} d \vec{\Omega}^{\prime}
\end{array}\right.
$$

Which, after further calculations, leads to:

$$
\operatorname{arcc} \varphi_{g}=\sum_{g^{\prime}}\left(\frac{1}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}\right)+\left(1-\frac{B}{\Sigma_{t}^{g}} \arctan \frac{B}{\Sigma_{t}^{g} \Sigma_{s, 1}^{g^{\prime} \rightarrow g}}\right) \frac{\vec{B} \cdot \vec{j}_{g^{\prime}}}{i B^{2}}\right)
$$

Thus, a coupling is introduced between the groups. The neutron balance is obtained by integrating Eq. (14.11) angularly, i.e.:

$$
i \vec{B} \cdot \vec{j}_{g}+\Sigma_{t}^{g} \varphi_{g}=\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}
$$

Hence, the term $\vec{B} \cdot \vec{j}_{g^{\prime}}$ is removed from the coupled flux equations:

$$
\varphi_{g}=\sum_{g^{\prime}}\left(\frac{1}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\left(\sum_{g^{\prime}} \Sigma_{0}^{g^{\prime} \rightarrow g} \varphi_{g^{\prime}}\right)-\left(1-\frac{B}{\Sigma_{t}^{g}} \arctan \frac{B}{\Sigma_{t}^{g}} \Sigma_{s, 1}^{g^{\prime} \rightarrow g}\right) \frac{\sum_{g^{\prime \prime}} \Sigma_{0}^{g^{\prime \prime} \rightarrow g^{\prime}} \varphi_{g^{\prime \prime}}-\Sigma_{t}^{g^{\prime}} \varphi_{g^{\prime}}}{B^{2}}\right)
$$

Some more mathematical computations result in the diffusion coefficient:

$$
D_{g} \equiv \frac{1}{B} \frac{\left(1-\frac{\Sigma_{i}^{g}}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\right)}{\arctan \frac{B}{\Sigma_{t}^{g}}}\left(1+\sum_{g^{\prime}} \Sigma_{s, 1}^{g^{\prime} \rightarrow g} \frac{\varphi_{g^{\prime}}}{\varphi_{g}} D_{g^{\prime}}\right)=D_{g, B_{0}}\left(1+\sum_{g^{\prime}} \Sigma_{s, 1}^{g^{\prime} \rightarrow g} \frac{\varphi_{g^{\prime}}}{\varphi_{g}} D_{g^{\prime}}\right)
$$

### 14.4.5.2 Finite Medium

Using the integral form of the Boltzmann equation as discussed in Chap. 8, the flux equation for a finite geometry as a function of that for an infinite geometry is established thanks to Benoist's method. We recall the flux equation in its volume integral form for a time-independent situation:

$$
\begin{aligned}
\Phi(\vec{r}, v,) & =\int_{V} d^{3} r^{\prime} q\left(\vec{r}^{\prime}, v,\right) \frac{e^{-\overline{\Sigma_{\ell} \ell}}}{4 \pi \ell^{2}} \\
& =\int_{V} d^{3} r^{\prime} \frac{e^{-\overline{\Sigma_{\ell} \ell}}}{4 \pi \ell^{2}}\left[\begin{array}{l}
\chi(v) \int_{0}^{\infty} d v^{\prime} v \Sigma_{f}\left(\vec{r}^{\prime}, v^{\prime}\right) \Phi\left(\vec{r}, v^{\prime},\right) \\
+\int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}^{\prime}, v^{\prime} \rightarrow v\right) \Phi\left(\vec{r}, v^{\prime},\right)+S\left(\vec{r}^{\prime}, v,\right)
\end{array}\right]
\end{aligned}
$$

which is written as follows with the Peierls operator:

$$
\Phi(\vec{r}, \quad v,)=K\left[\Sigma_{s} \Phi+\chi v \Sigma_{f} \Phi+S\right] \equiv K\left[\Sigma_{s} \Phi+Q\right]
$$

In the absence of independent sources, the source is assumed to be factorizable as the product of a macroscopic function $\Psi(\vec{r})$ and the source in an infinite lattice $Q_{\infty}(\vec{r}):$

$$
Q(\vec{r})=\Psi(\vec{r}) Q_{\infty}(\vec{r})
$$

The flux in an infinite lattice is expressed as:

$$
\Phi_{\infty}(\vec{r}, v,)=K_{\infty}\left[\Sigma_{s} \Phi_{\infty}+Q_{\infty}\right]
$$

Furthermore, it can be assumed that the operator $K[]$, which has an integral over a finite volume, can be prolonged such that it coincides with $K_{\infty}$ [] on the reactor. The infinite lattice flux equation is multiplied on both sides by $\Psi(\vec{r})$, and the resulting equation is subtracted term-wise from the flux equation for a finite
geometry. Further, a zero term is added such that the following grouping of terms can be applied:

$$
\begin{aligned}
\Phi(\vec{r}, v)-\psi(\vec{r}) \Phi_{\infty}(\vec{r}, v)= & K\left[\Sigma_{s} \Phi+\psi(\vec{r}) Q_{\infty}\right]-\psi(\vec{r}) K\left[\Sigma_{s} \Phi_{\infty}+Q_{\infty}\right] \\
& +\underbrace{K\left[\Sigma_{s} \psi(\vec{r}) \Phi_{\infty}\right]-K\left[\Sigma_{s} \psi(\vec{r}) \Phi_{\infty}\right]}_{0} \\
= & K\left[\Sigma_{s} \Phi-\Sigma_{s} \psi(\vec{r}) \Phi_{\infty}\right]-\psi(\vec{r}) K\left[\Sigma_{s} \Phi_{\infty}+Q_{\infty}\right] \\
& +K\left[\psi(\vec{r}) Q_{\infty}+\Sigma_{s} \psi(\vec{r}) \Phi_{\infty}\right]
\end{aligned}
$$

The last two terms are written in the integral form with $d^{3} r^{\prime}=\ell^{2} d \ell d \vec{\Omega}$ :

$$
\begin{aligned}
& \int_{\ell=0}^{+\infty} d \ell \frac{e^{-\Sigma_{, \ell}}}{4 \pi} \int_{4 \pi} d \vec{\Omega}(\underbrace{\chi(v) \int_{0}^{\infty} d v^{\prime} \nu \Sigma_{f}\left(\vec{r}^{\prime}, \nu^{\prime}\right) \Phi_{\infty}\left(\vec{r}^{\prime}, v^{\prime}\right)}_{Q_{\infty}\left(\vec{r}^{\prime}, v\right)}+\int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}^{\prime}, v^{\prime} \rightarrow v\right) \Phi_{\infty}\left(\vec{r}^{\prime}, \nu^{\prime}\right)) \\
& \times\left(\psi\left(\vec{r}^{\prime}\right)-\psi(\vec{r})\right)
\end{aligned}
$$

which by integration by parts for variable $\ell$ simplifies as follows with $\overline{\Sigma_{t} \ell^{\prime}} \equiv \int_{\ell^{\prime \prime}=0}^{\ell^{\prime \prime}=\left|\vec{r}-\vec{r}^{\prime \prime}\right|} \Sigma_{t}\left(\vec{r}-\ell^{\prime \prime} \bar{\Omega}, v\right) d \ell^{\prime \prime}:$
$\left[(\psi(\vec{r})-\psi(\vec{r})) \int_{\ell=\ell}^{+\infty} d \ell^{\frac{e^{-\overline{z_{,} \ell}}}{4 \pi}} \int_{4 \pi} d \overrightarrow{\Omega^{\prime}}\left(Q_{\infty}\left(\vec{r}^{\prime \prime}, v\right)+\int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}^{\prime \prime}, v^{\prime} \rightarrow v\right) \Phi_{\infty}\left(\vec{r}^{\prime \prime}, \nu^{\prime}\right)\right)\right]_{\ell=0}^{\ell=+\infty}$
$-\int_{4 \pi} d \overrightarrow{\Omega^{\prime}} \vec{\Omega}^{\prime} \cdot \int_{\ell=0}^{\ell=+\infty} d \overrightarrow{\ell g r a d} \psi \int_{\ell=\ell}^{+\infty} d \ell^{\prime} \frac{e^{-\overrightarrow{\Sigma_{\ell},}}}{4 \pi}\left(Q_{\infty}\left(\vec{r}^{\prime \prime}, v\right)+\int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}^{\prime \prime}, v^{\prime} \rightarrow v\right) \Phi_{\infty}\left(\vec{r}^{\prime \prime}, v^{\prime}\right)\right)$
At $\ell=0, \vec{r}=\overrightarrow{r^{\prime}}$, hence $\psi\left(\overrightarrow{r^{\prime}}\right)-\psi(\vec{r})=0$. Further, for $\ell=+\infty$, the exponential term tends towards 0 . Thus, the first integrated term is zero. For the second term with the gradient of the macroscopic form, the following flux equation is observed:

$$
\Phi_{\infty}\left(\vec{r}^{\prime}, v^{\prime}\right)=\int_{\ell^{\prime}=\ell}^{+\infty} d \ell^{\prime} \frac{-\overline{\Sigma_{l} \ell}}{4 \pi}\left(Q_{\infty}\left(\vec{r}^{\prime \prime}, v\right)+\int_{0}^{\infty} d v^{\prime} \Sigma_{S}\left(\vec{r}^{\prime \prime}, v^{\prime} \rightarrow v\right) \Phi_{\infty}\left(\vec{r}^{\prime \prime}, v^{\prime}\right)\right)
$$

Finally:

$$
\Phi(\vec{r}, v)-\psi(\vec{r}) \quad \Phi_{\infty}(\vec{r}, v)=K\left[\Sigma_{s} \Phi-\Sigma_{s} \psi(\vec{r}) \Phi_{\infty}\right]-K\left[\Phi_{\infty} \vec{\Omega} \cdot \overrightarrow{g r a d} \Psi\right]
$$

Benoist introduced the Peierls collision operator: $H[\Phi] \equiv K\left[\Sigma_{s} \Phi\right]$, which summarizes the previous equations as:

$$
\Phi(\vec{r}, v)-\psi(\vec{r}) \Phi_{\infty}(\vec{r}, v)=H\left[\Phi-\psi(\vec{r}) \Phi_{\infty}\right]-K\left[\Phi_{\infty} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Psi\right]
$$

or:

$$
\Phi(\vec{r}, v)=\psi(\vec{r}) \quad \Phi_{\infty}(\vec{r}, v)-\frac{1}{1-H}\left[K\left[\Phi_{\infty} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Psi\right]\right]
$$

where $\frac{1}{1-H}$ [] is the inverse operator that can be decomposed into the form of a Neumann series for successive collisions:

$$
\frac{1}{1-H}[] \equiv \sum_{n=0}^{+\infty} H^{n}[]
$$

A similar calculation can be performed for the current such that:

$$
\vec{J}(\vec{r}, v)=\psi(\vec{r}) \overrightarrow{J_{\infty}}(\vec{r}, v)-\frac{1}{1-H}\left[K \vec{\Omega}\left[\Phi_{\infty} \vec{\Omega} \cdot \overrightarrow{\operatorname{grad}} \Psi\right]\right]
$$

This result can be written with the Green function $G\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime} ; \vec{r}, \vec{\Omega}, v\right)$ corresponding to the number of neutrons at $(\vec{r}, \vec{\Omega}, v)$ produced by a neutron emitted at $\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime}\right)$ in the phase space:

$$
\begin{aligned}
& \Phi(\vec{r}, v)=\psi(\vec{r}) \Phi_{\infty}(\vec{r}, v) \\
& -\int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} v^{\prime} d v^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{\infty} d^{3} r^{\prime} G\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime} ; \vec{r}, \vec{\Omega}, v\right) n\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime}\right) \vec{\Omega}^{\prime} \cdot \overrightarrow{\operatorname{grad}} \Psi\left(\vec{r}^{\prime}\right)
\end{aligned}
$$

If the macroscopic function varies slowly in space, the Peierls operator can be commuted with the gradient (which is a result obtained by expanding $\overrightarrow{\operatorname{grad}} \Psi(\vec{r})$ around $\vec{r}$ ), and the result is expressed simply as:

$$
\left\{\begin{array}{l}
\Phi(\vec{r}, v)=\psi(\vec{r}) \Phi_{\infty}(\vec{r}, v)-\vec{\Phi}_{1}(\vec{r}, v) \cdot \overrightarrow{\operatorname{grad}} \Psi(\vec{r}) \\
\vec{\Phi}_{1}(\vec{r}, v) \equiv \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} v^{\prime} d v^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{\infty} d^{3} r^{\prime} G\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime} ; \vec{r}, \vec{\Omega}, v\right) n\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime}\right) \vec{\Omega}^{\prime}
\end{array}\right.
$$

$$
\left\{\begin{array}{l}
\vec{J}(\vec{r}, v) \cdot \vec{\Omega}_{k}=\psi(\vec{r}) \overrightarrow{J_{\infty}}(\vec{r}, v) \cdot \vec{\Omega}_{k}-\sum_{k^{\prime}} J_{1, k, k^{\prime}}(\vec{r}, v) \overrightarrow{\operatorname{grad}} \Psi(\vec{r}) \cdot \vec{\Omega}_{k} \\
J_{1, k, k^{\prime}}(\vec{r}, v) \equiv \int_{4 \pi} d \vec{\Omega} \int_{0}^{\infty} v^{\prime} d v^{\prime} \int_{4 \pi} d \vec{\Omega}^{\prime} \int_{\infty}^{3} d^{3} r^{\prime} G\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime} ; \vec{r}, \vec{\Omega}, v\right) n\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime}\right) \vec{\Omega}_{k} \cdot \vec{\Omega}_{k^{\prime}}
\end{array}\right.
$$

An important consequence of the finite medium is that the flux can no longer be factorized due to the correction of the gradient of the macroscopic flux. If the macroscopic flux has a large buckling, then $\overrightarrow{\operatorname{grad}} \Psi(\vec{r})$ should be calculated as a function of Taylor series expansion with respect to the buckling, and the corresponding integrals can be calculated in the manner used by V. C. Deniz in 1965. The integration kernel $G\left(\vec{r}^{\prime}, \vec{\Omega}^{\prime}, v^{\prime} ; \vec{r}, \vec{\Omega}, v\right)$ can be calculated analytically for simple cases. ${ }^{39}$

### 14.4.6 Spatial Homogenization with Leakage

Engineering calculations in neutron physics are carried out with the diffusion approximation and the main question is how to homogenize the diffusion

[^306]
(Courtesy Lam Hime)
coefficient with respect to the space variable. Indeed, homogeneous cross sections for an assembly are usually obtained by weighting the reaction rates computed in transport theory on a heterogeneous geometry with the computational volumes. However, for the diffusion coefficient, the most straightforward approach is to apply the same method to the mean free path:
$$
D_{B=0, \text { isotropic }}^{P_{0}} \equiv \sum_{i} \frac{V_{i} \Phi_{i} \frac{1}{3 \Sigma_{l, i}}}{\sum_{i} V_{i} \Phi_{i}}
$$

This definition corresponds to the definition of $D_{B=0, \text { isotropic }}^{P_{0}}$ for the diffusion coefficient, i.e. the order 0 for the expansion of the scattering cross section (thus, the index $P_{0}$ ) obtained in an infinite lattice without leakage (thus the index $B=0$ ) and which is applied isotropically in all directions (hence, the index "isotropic"). Yet, soon enough, it was realized that such a diffusion coefficient, which was discussed in the chapter on the diffusion approximation and on Fick's law, led to results that poorly represented the expected physics, or were even catastrophic for few-group calculations. During the design of the 3D $S P_{n}$ code COCAGNE at $E D F$, these disappointing results were jokingly referred to as the "casserole" (referring both to the shape of a pot used for cooking and, jokingly, the French slang for a "mistake"). Use of these diffusion coefficients for two-energy groups obtained through this weighting method did not result in correct propagation of neutrons in the core, decoupling the various zones of the core such that all the power was produced by the fresh assemblies located at the periphery (the second layer of assemblies from the center for fuel patterns with weak fluence). This resulted in the characteristic "saucepan" shape of the radial traverses of the core.

The problem was solved by using a second approach, which considered that the collision assumed to be isotropic in the center of mass was too coarse for water reactors. Thus, the diffusion coefficient is defined using the transport cross sections, instead of the total cross sections, i.e.:

$$
D_{B=0, \text { isotropic }}^{P_{1}} \equiv \sum_{i} \frac{V_{i} \Phi_{i} \frac{1}{3 \Sigma_{t r, i}}}{\sum_{i} V_{i} \Phi_{i}}=\sum_{i} \frac{V_{i} \Phi_{i} \frac{1}{3\left(\Sigma_{t, i}-\Sigma_{s, 1}\right)}}{\sum_{i} V_{i} \Phi_{i}}
$$

Nonetheless, the use of such a coefficient, although it improved the solution, did not solve the problem totally. Pierre Benoist proposed to account for collision probabilities $P_{i j}$ in the calculation of the diffusion coefficient, called the Benoist diffusion coefficient:

$$
D_{\text {Benoist }}=D_{B, \text { isotropic }}^{P_{1}} \equiv \sum_{i} \sum_{j} \frac{V_{i} \Phi_{i} P_{i j} \frac{1}{3 \Sigma_{t r, j}}}{\sum_{i} V_{i} \Phi_{i}}
$$

It was previously seen that this new diffusion coefficient can be expressed in terms of $D_{B=0, \text { isotropic }}^{P_{0}}$ :

$$
D_{\text {Benoist }}=\frac{1}{B} \frac{\left(1-\frac{\Sigma_{t}}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\right)}{\arctan \frac{B}{\Sigma_{t}}}=\frac{1}{3 \Sigma_{t} \gamma}=\frac{D_{B=0, \text { isotropic }}^{P_{0}}}{\gamma}
$$

With this calculation, the dimensionless coefficient $\gamma$ can be evaluated:

$$
\gamma \equiv \frac{B}{3} \frac{\arctan \frac{B}{\Sigma_{t}}}{\left(1-\frac{\Sigma_{t}}{B} \arctan \frac{B}{\Sigma_{t}^{g}}\right)}
$$

Hence, the infinite lattice calculation is performed in transport theory and made critical by superposing leakage characterized by the critical buckling (the leakage term can be positive or negative). The diffusion coefficient is then corrected by the coefficient $\gamma$ that accounts for the buckling. This correction is significant for few energy groups. The French APOLLO1 code used this method (Fig. 14.20).


Fig. 14.20 Effect of diffusion coefficient on power distribution (from COCAGNE calculations performed by Fabrice Hoareau in 2013).

In 1964, Benoist proposed an improvement in homogenization techniques using a directional approach. In a Cartesian geometry, let $k \in\{x, y\}$, and in a cylindrical geometry, $k \in\{r, z\}$. The directional diffusion coefficient is defined as:

$$
D_{\text {Benoist }, k}=\sum_{i} \sum_{j} \frac{V_{i} \Phi_{i} P_{i j, k} \frac{1}{3 \Sigma_{t, j}}}{\sum_{i} V_{i} \Phi_{i}}
$$

where $P_{i j, k}$ is the probability of directional first collisions.
The directional probabilities in direction $k$ are given by:

$$
P_{i j, k}=\frac{3 \Sigma_{t, j}}{V_{i}} \int_{\forall j, V_{j}} d \vec{r} \int_{V_{i}} d \overrightarrow{r^{\prime}} \Omega_{k}^{2} \frac{e^{-\overline{\Sigma_{l} R}}}{4 \pi R^{2}} \cos (\vec{B} \cdot \vec{R})
$$

where $\vec{R}=\vec{r}-\overrightarrow{r^{\prime}}=R \vec{\Omega}$. It can be noted that the integral on $\vec{r}$ is performed for all cells in the lattice of the same type $j$ due to the summation sign on the $j$ indices, while the integral on $\overrightarrow{r^{\prime}}$ applies only for cell $i$. The directional probabilities satisfy:

$$
\frac{V_{i} P_{i j, k}}{\Sigma_{t, j}}=\frac{V_{j} P_{j i, k}}{\Sigma_{t, i}}
$$

And:

$$
\begin{aligned}
\sum_{j} P_{i j, k} & =\sum_{j} \frac{3}{V_{i}} \int_{\infty} d \vec{r} \Sigma_{t, j} \int_{V_{i}} d \overrightarrow{r^{\prime}} \Omega_{k}^{2} \frac{e^{-\overline{\Sigma_{t} R}}}{4 \pi R^{2}} \cos (\vec{B} \cdot \vec{R}) \\
& =\frac{3}{V_{i}} \int_{V_{i}} d \overrightarrow{r^{\prime}} \int_{4 \pi} \frac{\Omega_{k}^{2}}{4 \pi} d \Omega \int_{R=0}^{R=\infty} d \vec{r} \Sigma_{t}(\vec{r}) e^{-\overline{\Sigma_{l} R}} \cos (\vec{B} \cdot \vec{R})
\end{aligned}
$$

Since $\left\{\begin{array}{l}\int_{4 \pi} \frac{\Omega_{z}^{2}}{4 \pi} d \Omega=\int_{0}^{\frac{\pi}{2}} \sin \theta \cos ^{2} \theta d \theta=\left[-\frac{\cos ^{3} \theta}{3}\right]_{0}^{\frac{\pi}{2}}=\frac{1}{3} \\ \int_{4 \pi}^{\frac{\Omega_{r}^{2}}{2}} d \Omega=\int_{0}^{\frac{\pi}{2}} \sin \theta \frac{\sin ^{2} \theta}{2} d \theta=\int_{0}^{\frac{\pi}{2}} \sin \theta \frac{1-\cos ^{2} \theta}{2} d \theta=\frac{1}{2}-\frac{1}{6}=\frac{1}{3}\end{array}\right.$
And also, integrating by parts

$$
\int_{R=0}^{R=\infty} d \vec{r} \Sigma_{t}(\vec{r}) e^{-\overline{\Sigma_{l} R}} \cos (\vec{B} \cdot \vec{R})=1-\vec{B} \cdot \vec{R} \int_{R=0}^{R=\infty} d \vec{r} e^{-\overline{\Sigma_{l} R}} \sin (\vec{B} \cdot \vec{R})
$$

Hence:

$$
\sum_{j} P_{i j, k}=1-\vec{B} \cdot \vec{R} \int_{R=0}^{R=\infty} d \vec{r} e^{-\overline{\Sigma_{l} R}} \sin (\vec{B} \cdot \vec{R})=1-O\left(B^{2}\right)
$$

The collision probabilities are simply normalized to 1 if the buckling term is expanded at order 1.

The Taylor expansion of the buckling at order 0 (which is equivalent to setting $P_{i j, k}=1$ in the equations) results in a "streaming" problem, i.e. neutrons leak in a preferential direction (e.g. into the gas channels of gas reactors or into voided water channels in water reactors or sodium-cooled fast reactors). In this case, the diffusion coefficient in the direction parallel to the voided channels has an infinite value since the total cross section is zero. This problem can be avoided by means of calculations in voided regions (by setting a density limit for instance), but this implies a patch-up solution since diffusion theory is no longer valid in configurations in which neutrons can be transported far away from their source. Even if filled with sodium, which is mostly "transparent" for neutrons, the axial streaming effect is still significant. A "pragmatic" solution consists in using an isotropic diffusion coefficient defined as the average of the directional diffusion coefficients:

$$
D_{\text {Benoist }, \text { isotropic }}=\sum_{i} \sum_{j} \frac{V_{i} \Phi_{i}\left\langle P_{i j}\right\rangle \frac{1}{3 \Sigma_{t, j}}}{\sum_{i} V_{i} \Phi_{i}}
$$

where the average directional probability is applied $\left\langle P_{i, j}\right\rangle \equiv \frac{1}{2} \sum_{k} P_{i j, k}$.
In sodium reactors, accurate calculation of the void effect is essential due to the closed geometry of hexagonal cans. Studies in the 1980s showed that use of an isotropic Benoist coefficient weakly underestimated (by some 50 pcm ) the streaming effect, i.e. at most $1 \%$ of the total sodium void effect. In water reactors, voiding of a channel does not cause any problems thanks to the open geometry of the assemblies.

In 1981, Benoist proposed ${ }^{40}$ an extension of directional probabilities to more accurately take in to account the streaming effect by adopting a logarithmic expansion of the buckling term, the lowest order retaining physical meaning, i.e. a finite directional diffusion coefficient in the direction of the voided channels. He carried out analytical calculations for the terms included in the directional diffusion coefficient for geometries with pins in a square-pitch lattice $(P W R)$ and in triangular lattices (VVER, fast reactors).

[^307]Fig. 14.21 Slab reactor


### 14.4.7 Equivalence for Slab Reactors

The non-consistency effect has been studied in a mathematical framework for some simple geometries. C. Robert studied ${ }^{41}$ the non-consistency effect on the theoretical calculation of the diffusion coefficient in a slab lattice. He proved that there exists an exact equivalence allowing the calculation of a reactor in diffusion theory by preserving the flux and currents at the interfaces with respect to transport theory. Such an approach has been applied successfully to 1D radial geometries for fast reactors. Let us consider a slab lattice surrounded by a vacuum (Fig. 14.21):

Each slab is sub-divided into regions indexed by $j$ for constant properties. A position in a region $j$ is located by $\tau_{j}$ its local abscissa coordinate with respect to the center of the region and by $x_{i}$ in the common frame (Fig. 14.22).

The even (or symmetric) flux and odd (anti-symmetric) flux are defined in each region using the formulation which was illustrated in the chapter on the Boltzmann equation:

$$
\begin{aligned}
& \Phi_{j}^{+}\left(\tau_{j}, \mu\right)=\frac{1}{2}\left[\Phi_{j}\left(\tau_{j}, \mu\right)+\Phi_{j}\left(-\tau_{j}, \mu\right)\right] \\
& \Phi_{j}^{-}\left(\tau_{j}, \mu\right)=\frac{1}{2}\left[\Phi_{j}\left(\tau_{j}, \mu\right)-\Phi_{j}\left(-\tau_{j}, \mu\right)\right]
\end{aligned}
$$

and the corresponding currents are:

[^308]Fig. 14.22 Regions in a slab


$$
\begin{aligned}
& J_{j}^{+}\left(\tau_{j}\right)=\int_{-1}^{+1} \mu \Phi_{j}^{+}\left(\tau_{j}, \mu\right) d \mu \\
& J_{j}^{-}\left(\tau_{j}\right)=\int_{-1}^{+1} \mu \Phi_{j}^{-}\left(\tau_{j}, \mu\right) d \mu
\end{aligned}
$$

These quantities can be defined in both transport (index $t$ ) and diffusion (index $d$ ). It should be pointed out that by construction, the anti-symmetric current is even. In diffusion theory, the currents are related to the flux by Fick's law:

$$
J_{j, d}^{+}\left(\tau_{j}\right)=-D_{j}\left|\overrightarrow{\operatorname{grad}} \Phi_{j, d}^{+}\left(\tau_{j}\right)\right| \quad \text { and } \quad J_{j, d}^{-}\left(\tau_{j}\right)=-D_{j}\left|\overrightarrow{\operatorname{grad}} \Phi_{j, d}^{-}\left(\tau_{j}\right)\right|
$$

With these notations, ${ }^{42}$ the diffusion equation in region $j$ is expressed as:

$$
-D_{j} \frac{d^{2} \Phi_{j, d}}{d \tau_{j}^{2}}+\left(\Sigma_{t j, d}-\Sigma_{s j, d}\right) \Phi_{j, d}=\frac{v \Sigma_{f j, d} \Phi_{j, d}}{k_{e f f, d}}
$$

In transport and diffusion, the even and odd extrapolation distances can be defined such that they are dimensionless:

[^309]$$
\Lambda_{j}^{+}=\frac{\Phi_{j}^{+}}{J_{j}^{+}}=\frac{\Phi_{j}\left(\delta_{j}\right)+\Phi_{j}\left(-\delta_{j}\right)}{J_{j}\left(\delta_{j}\right)-J_{j}\left(-\delta_{j}\right)} \quad \text { and } \quad \Lambda_{j}^{-}=\frac{\Phi_{j}^{-}\left(\delta_{j}\right)}{J_{j}^{-}\left(\delta_{j}\right)}=\frac{\Phi_{j}\left(\delta_{j}\right)-\Phi_{j}\left(-\delta_{j}\right)}{J_{j}\left(\delta_{j}\right)+J_{j}\left(-\delta_{j}\right)}
$$

Setting $B_{j}^{2}=\left(\Sigma_{t j, d}-v \Sigma_{f j, d} / k_{e f f, d}-\Sigma_{s j, d}\right) / D_{j}$, the diffusion flux and currents can be determined using the eigenfunctions of the buckling term in finite slab geometry:

$$
\begin{array}{rlrl} 
& \Phi_{j, d}\left(\tau_{j}\right) & =\varphi_{j} \cos \left(B_{j} \tau_{j}\right)+\psi_{j} \sin \left(B_{j} \tau_{j}\right) \\
& \text { and } & J_{j, d}\left(\tau_{j}\right) & =D_{j} B_{j}\left[\varphi_{j} \sin \left(B_{j} \tau_{j}\right)-\psi_{j} \cos \left(B_{j} \tau_{j}\right)\right]
\end{array}
$$

Thus, the symmetric (cosine) and anti-symmetric (sine) components of the flux and current can be easily identified and the diffusion extrapolation distances evaluated:

$$
\Lambda_{j, d}^{+}=\frac{1}{D_{j} B_{j} \tan \left(B_{j} \delta_{j}\right)} \quad \text { and } \quad \Lambda_{j, d}^{-}=-\frac{\tan \left(B_{j} \delta_{j}\right)}{D_{j} B_{j}}
$$

There is an exact equivalence which, with a judicious choice of diffusion coefficient, leads to the same extrapolation distance as in transport theory for $k_{\text {eff }}$, ${ }_{d}=k_{\text {eff }, t}$. Further, it can be shown that the parameter $B_{j}^{2}$ satisfies $\left|B_{j}\right|<\pi /\left(2 \delta_{j}\right)$, the geometrical buckling in the region $j$, if $B_{j}$ is real. Furthermore, if the following boundary conditions are set on the periphery of the reactor:

Boundary conditions at the limits of the reactor:

$$
\begin{equation*}
\frac{\Phi_{j, d}\left(-b_{1}\right)}{J_{j, d}\left(-b_{1}\right)}=\frac{\Phi_{j, f}\left(-b_{1}\right)}{J_{j, f}\left(-b_{1}\right)} \quad \text { and } \quad \frac{\Phi_{j, d}\left(+b_{n}\right)}{J_{j, d}\left(+b_{n}\right)}=\frac{\Phi_{j, f}\left(+b_{n}\right)}{J_{j, f}\left(+b_{n}\right)} \tag{14.12}
\end{equation*}
$$

Then, the fluxes and currents at the interfaces of all the regions and at the limits of the reactor are strictly equal in both diffusion and transport theories. For this result, the diffusion flux is constructed as:

Transport-equivalent diffusion flux:

$$
\begin{equation*}
\Phi_{j, d}\left(\tau_{j}\right)=\frac{1}{2}\left[\frac{\Phi_{j, t}\left(+\delta_{j}\right)+\Phi_{j, t}\left(-\delta_{j}\right)}{\cos \left(B_{j, t} \delta_{j}\right)} \cos \left(B_{j, t} \tau_{j}\right)+\frac{\Phi_{j, t}\left(+\delta_{j}\right)-\Phi_{j, t}\left(-\delta_{j}\right)}{\sin \left(B_{j, t} \delta_{j}\right)} \sin \left(B_{j, t} \tau_{j}\right)\right] \tag{14.13}
\end{equation*}
$$

with the particular value of $B_{j, t}$, which satisfies the diffusion equation written with the multiplication coefficient $k_{\text {eff }, t}$ calculated in transport theory (and not in diffusion):

$$
B_{j, t}^{2}=\frac{\left(\Sigma_{t j, d}-\frac{v \Sigma_{f j, d}}{k_{e f f, t}}-\Sigma_{s j, d}\right)}{D_{j}}
$$

By construction, the flux from Eq. (14.13) satisfies the diffusion equation with $k_{\text {eff }, t}$ :

$$
-D_{j} \frac{d^{2} \Phi_{j, d}}{d \tau_{j}^{2}}+\left(\Sigma_{t j, d}-\Sigma_{s j, d}\right) \Phi_{j, d}=\frac{v \Sigma_{f j, d} \Phi_{j, d}}{k_{e f f, t}}
$$

Moreover, it is also continuous, as well as the corresponding current, and by construction verifies the following equations:

$$
\Phi_{j, d}\left(\delta_{j}\right)=\Phi_{j, t}\left(\delta_{j}\right) \quad \text { and } \quad \Phi_{j, d}\left(-\delta_{j}\right)=\Phi_{j, t}\left(-\delta_{j}\right)
$$

If $D_{j}, \Sigma_{t j, d}, v \Sigma_{f j, d}$ and $\Sigma_{s j, d}$ are chosen such that:

$$
\begin{gathered}
\Lambda_{j, d}^{+}=\frac{1}{D_{j} B_{j, t} \tan \left(B_{j, t} \delta_{j}\right)}=\frac{\Phi_{j, t}\left(\delta_{j}\right)+\Phi_{j, t}\left(-\delta_{j}\right)}{J_{j, t}\left(\delta_{j}\right)-J_{j, t}\left(-\delta_{j}\right)} \\
\Lambda_{j, d}^{-}=-\frac{\tan \left(B_{j} \delta_{j}\right)}{D_{j} B, t_{j, t}}=\frac{\Phi_{j, t}\left(\delta_{j}\right)-\Phi_{j, t}\left(-\delta_{j}\right)}{J_{j, t}\left(\delta_{j}\right)+J_{j, t}\left(-\delta_{j}\right)}
\end{gathered}
$$

the diffusion current is expressed in terms of the transport current as:

$$
\begin{aligned}
J_{j, d}\left(\tau_{j}\right)=-D_{j} \frac{\partial \Phi_{j, d}}{\partial \tau_{j}} & =\frac{D_{j}}{2}\left[\frac{\Phi_{j, t}\left(+\delta_{j}\right)+\Phi_{j, t}\left(-\delta_{j}\right)}{\cos \left(B_{j, t} \delta_{j}\right)} B_{j, t} \sin \left(B_{j, t} \tau_{j}\right)-\frac{\Phi_{j, t}\left(+\delta_{j}\right)-\Phi_{j, t}\left(-\delta_{j}\right)}{\sin \left(B_{j, t} \delta_{j}\right)} B_{j, t} \cos \left(B_{j, t} \tau_{j}\right)\right] \\
& =\frac{1}{2}\left[\frac{J_{j, t}\left(\delta_{j}\right)+J_{j, t}\left(-\delta_{j}\right)}{\cos \left(B_{j, t} \delta_{j}\right)} \cos \left(B_{j, t} \tau_{j}\right)+\frac{J_{j, t}\left(\delta_{j}\right)-J_{j, t}\left(-\delta_{j}\right)}{\sin \left(B_{j, t} \delta_{j}\right)} \sin \left(B_{j, t} \tau_{j}\right)\right]
\end{aligned}
$$

It can be observed that: $J_{j, d}\left(\delta_{j}\right)=J_{j, t}\left(\delta_{j}\right)$ and $J_{j, d}\left(-\delta_{j}\right)=J_{j, t}\left(-\delta_{j}\right)$
Assuming that $\left|B_{j, t}\right|<\pi /\left(2 \delta_{j}\right)$, the diffusion flux is expressed as:

$$
\Phi_{j, d}\left(\tau_{j}\right)=\frac{\Phi_{j, t}\left(+\delta_{j}\right) \sin \left(B_{j, t}\left(\delta_{j}+\tau_{j}\right)\right)+\Phi_{j, t}\left(-\delta_{j}\right) \sin \left(B_{j, t}\left(\delta_{j}-\tau_{j}\right)\right)}{\sin \left(2 B_{j, t} \delta_{j}\right)}
$$

which shows that the flux has the same sign for all regions of the slab. It can also be shown that the extrapolation distances for diffusion and transport are equal for each region $j$. Subsequently, the flux to current ratio being also equal at the reactor boundaries leads to the construction of a diffusion flux that satisfies the fact that the transport and diffusion flux and currents are equal at the interfaces. Equivalence is thus verified if the following equations are satisfied:

$$
\frac{1}{D_{j} B_{j, t} \tan \left(B_{j, t} \delta_{j}\right)}=\Lambda_{j, t}^{+} \quad \text { and } \quad-\frac{\tan \left(B_{j, t} \delta_{j}\right)}{D_{j} B_{j, t}}=\Lambda_{j, t}^{-}
$$

by adjusting the four neutron quantities $D_{j}, \Sigma_{t j, d}, v \Sigma_{f j, d}$, and $\Sigma_{s j, d}$. From both equations, the following equations are deduced:

$$
\frac{1}{\left(D_{j} B_{j, t}\right)^{2}}=-\Lambda_{j, t}^{+} \Lambda_{j, t}^{-} \quad \text { and } \quad \tan ^{2}\left(B_{j} \delta_{j}\right)=-\frac{\Lambda_{j, t}^{-}}{\Lambda_{j, t}^{+}}
$$

If $\Lambda_{j, t}^{+}$and $\Lambda_{j, t}^{-}$are of opposite signs, $B_{j, t}$ is real and due to $\left|B_{j, t}\right|<\pi /\left(2 \delta_{j}\right)$, we obtain:

$$
B_{j, t}=\frac{1}{\delta_{j}} \arctan \sqrt{\left|\frac{\Lambda_{j, t}^{-}}{\Lambda_{j, t}^{+}}\right|} \quad \text { and } \quad D_{j}=\operatorname{sign}\left(\Lambda_{j, t}^{+}\right) \frac{\delta_{j}}{\sqrt{\left|\Lambda_{j, t}^{-} \Lambda_{j, t}^{+}\right|} \arctan \sqrt{\left|\frac{\Lambda_{j, t}^{-}}{\Lambda_{j, t}^{+}}\right|}}
$$

It can be pointed out that if $\Lambda_{j, t}^{+}$is negative, $D_{j}$ is also negative, which means that $\Sigma_{t j, d}-\Sigma_{s j, d}-v \Sigma_{f j, d} / k_{e f f, t}=D_{j} B_{j, t}^{2}<0$, and that the region is over-multiplying. Otherwise, the region is sub-multiplying and the second flux derivative is negative. If $\Lambda_{j, t}^{+}$and $\Lambda_{j, t}^{-}$are of the same sign, $B_{j, t}$ is a purely imaginary, and thus:
$\operatorname{th}^{2}\left(\left\|B_{j}\right\| \delta_{j}\right)=\frac{\Lambda_{j, t}^{-}}{\Lambda_{j, t}^{+}} \quad$ for which the solution exists only if: $\quad\left|\Lambda_{j, t}^{-}\right|<\left|\Lambda_{j, t}^{+}\right|$
Under this condition: $B_{j, t}=\frac{i}{\delta_{j}} \operatorname{Argth} \sqrt{\frac{\Lambda_{j, t}^{-}}{\Lambda_{j, t}^{+}}}$and $D_{j}=\operatorname{sign}\left(-\Lambda_{j, t}^{+}\right) \frac{\delta_{j}}{\sqrt{\Lambda_{j, t}^{-} \Lambda_{j, t}^{+}} \operatorname{Argth} \sqrt{\frac{\Lambda_{j, t}^{+}}{\Lambda_{j, t}^{+}}}}$
Once again, if $\Lambda_{j, t}^{+}$and $\Lambda_{j, t}^{-}$are both negative, the region is sub-multiplying. If $\Lambda_{j, t}^{+}$ and $\Lambda_{j, t}^{-}$are both positive, the region is over-multiplying. The case $\left|\Lambda_{j, t}^{-}\right|>\left|\Lambda_{j, t}^{+}\right|$ occurs when the current inside a region is zero. Hence, interfaces need only be located at positions where currents become zero so as to avoid the problem.

If $B_{j, t}$ and $D_{j}$ are known, the equation $B_{j, t}^{2}=\left(\Sigma_{t j, d}-\Sigma_{s j, d}-v \Sigma_{f j, d} / k_{e f f, t}\right) / D_{j}$ allows for two degrees of freedom. Therefore, we can choose to preserve the proportions between the transport and diffusion cross sections:

$$
\Sigma_{t j, d}=\alpha_{j} \Sigma_{t j, t}, \quad \Sigma_{s j, d}=\alpha_{j} \Sigma_{s j, t}, \quad v \Sigma_{f j, d}=\alpha_{j} v \Sigma_{f j, t}
$$

The proportionality coefficient is determined by:

$$
\alpha=\frac{\left(\Sigma_{t j, t}-\Sigma_{s j, t}-v \Sigma_{f j, t} / k_{e f f, t}\right)}{D_{j} B_{j, t}^{2}}
$$

It should be noted that such an approach is not iterative since the value of $\alpha$ is fixed as soon as $B_{j, t}$ and $D_{j}$ have been determined. It could have been decided to conserve the reaction rates between the transport and diffusion calculations, which would require an iterative method (a set of cross sections is chosen such that the criterion for $B_{j, t}^{2}$ is satisfied, the diffusion calculation that leads to the reaction rate $\Sigma_{d} \Phi_{d}$ is performed, and the latter is compared to $\Sigma_{t} \Phi_{t}$; the iterations are then carried out according to the degrees of freedom in order to adjust the reaction rates while preserving the criterion).

### 14.4.8 Equivalence by Conservation of Reaction Rates

Generalization of the previous problem results in conserving the reaction rates between the diffusion and the transport calculations. Starting with the integral Boltzmann equation, it can be shown imposing conservation of the reaction rates alone gives an infinite number of solutions. Hence, there is a degree of freedom, the normalization condition, which can be used to improve the result of the simplified calculation. It will later be shown that this normalization condition can be defined so as to conserve the flux at the interface of two assemblies for instance. After spatial homogenization and energy condensation, the cross sections obtained for a given reaction type $\kappa$ (total, fission, etc.) for an energy group $g$ and a volume $V_{j}$ are given by:

$$
\Sigma_{\kappa, j, t}^{g}=\frac{\int_{g} d E \int_{V_{j}} \Sigma_{\kappa, t}(\vec{r}, E) \Phi_{t}(\vec{r}, E) d \vec{r}}{\int_{g} d E \int_{V_{j}} \Phi_{t}(\vec{r}, E) d \vec{r}}
$$

The question remains of whether a transport calculation performed on the homogenization geometry (known as equivalent geometry) with the defined cross sections $\Sigma_{\kappa, j, t}^{g}$ leads to the same reaction rates as fine transport calculation. This is not the case since the transport equation is not linear with respect to the total cross section, which is used in a decreasing exponential term in the optical path. The conclusion is that equivalence is also required to ensure the conservation of reaction rates from fine transport to homogeneous transport, and a fortiori to diffusion calculations. In practical cases, equivalent diffusion cross sections are sought as:

$$
\Sigma_{i, j, d}^{g}=\mu_{i, j}^{g} \Sigma_{i, j, t}^{g}
$$

which has the property of conserving the reaction rates present in the definition of the neutron balance. The linear nature of the diffusion equation with respect to the diffusion coefficient suggests that the other cross sections may be corrected in the same way. Thus, if the same equivalence coefficient is applied to all cross sections, multiplicative correction of the diffusion coefficient does not modify the diffusion equation. Similarly, for the previous slab reactor situation, the solution to the problem is not unique. A closure relation is required to fix one solution: this is called a normalization condition. The possible normalization choices can be the conservation of the flux at the cell boundary ( $E D F$ method ${ }^{43}$ ) or set the equivalence coefficients to 1 for cells which are far ("at infinity") from the geometry being considered (these cells are called asymptotic cells since they are not influenced by the geometry being calculated). The choice to fix the normalization condition is not trivial. Indeed, the solution that conserves the reaction rates in the assembly for an infinite lattice can be chosen and when used in a core calculation, there are artificial discontinuities in the reaction rates at the interfaces of various homogeneous media: this is the non-consistency effect. This problem can be solved by allowing for an appropriate closure relation for instance by choosing peripheral cells far from heterogeneities (guide thimbles) in a $P W R$ assembly as the asymptotic cells. Another method is the use of discontinuity factors. The equivalence coefficients generally depend on the calculation mesh used in the diffusion calculation.

[^310]
(Courtesy Garzenne)

A simple method to deal with this problem, as proposed in the APOLLO2 code, is to set the same equivalence factors for all the cross sections in each region. This solution conserves the reaction rates as well as the absorption probabilities (both fission and slowing down) since:

$$
\left\{\begin{array}{l}
\Sigma_{a, j, d}^{g}=\mu_{j}^{g} \Sigma_{a, j, t}^{g} \\
\Sigma_{t, j, d}^{g}=\mu_{j}^{g} \Sigma_{a, j, t}^{g}
\end{array} \Rightarrow \frac{\Sigma_{a, j, d}^{g}}{\Sigma_{t, j, d}^{g}}=\frac{\Sigma_{a, j, t}^{g}}{\Sigma_{a, j, t}^{g}}\right.
$$

The conservation of the reaction rates per region is written as:

$$
\Sigma_{j, d}^{g} \Phi_{j, d}^{g}=\mu_{j}^{g} \Sigma_{j, t}^{g} \Phi_{j, d}^{g}=\Sigma_{j, t}^{g} \Phi_{j, t}^{g}
$$

meaning that the homogenized diffusion and transport flux are proportional: $\mu_{j}^{g} \Phi_{j, d}^{g}=\Phi_{j, t}^{g}$. In an infinite lattice, most codes achieve criticality on the geometry by superposing a leakage coefficient equal to $D_{t}^{g}=1 /\left(3 \Sigma_{t r, t}^{g}\right)$ in $P_{1}$ theory. A first approach consists in conserving the absorption balance and the leakage balance coherently for each cell. By substituting $\Phi_{j, t}^{g}$ by $\mu_{j}^{g} \Phi_{j, d}^{g}$ in the leakage balance, the following is obtained:

$$
\begin{aligned}
D_{j, d}^{g} B_{j}^{2} \Phi_{j, d}^{g}+\Sigma_{a, j, d}^{g} \Phi_{j, d}^{g} & =D_{j, t}^{g} B_{j}^{2} \Phi_{j, t}^{g}+\Sigma_{a, j, t}^{g} \Phi_{j, t}^{g} \\
& =\mu_{j}^{g}\left[\Phi_{j, d}^{g} B_{j}^{2} D_{j, t}^{g}+\Sigma_{a, j, t}^{g} \Phi_{j, t}^{g}\right] \Rightarrow D_{j, d}^{g}=\mu_{j}^{g} D_{j, t}^{g}
\end{aligned}
$$

It may be seen that in this approach, the diffusion coefficient should be corrected by the same factor as the other cross sections. It implies that the probabilities are conserved, even the leakage probability. The "leakage" ${ }^{44}$ term from the geometry can also be conserved using a mean diffusion coefficient by applying:

$$
\left(\sum_{j} V_{j} \Phi_{j, d}^{g}\right) D_{d}^{g}=\left(\sum_{j} V_{j} \Phi_{j, t}^{g}\right) D_{t}^{g}
$$

The conservation of the reaction rate corrected for the transport cross section is:

$$
\left(\sum_{j} V_{j} \Phi_{j, d}^{g}\right) \Sigma_{t r, d}^{g}=\left(\sum_{j} V_{j} \Phi_{j, t}^{g}\right) \Sigma_{t r, t}^{g}
$$

To conserve the relation $D_{d}^{g}=1 /\left(3 \Sigma_{t r, d}^{g}\right)$, the following must imperatively be satisfied:

[^311]$$
D_{d}^{g}=D_{t}^{g} \quad \text { and } \quad \sum_{t r, d}^{g}=\sum_{t r, t}^{g}
$$

Thus:

$$
\sum_{j} V_{j} \boldsymbol{\Phi}_{j, d}^{g}=\sum_{j} V_{j} \boldsymbol{\Phi}_{j, t}^{g}
$$

Using the proportionality between the homogenized transport flux and the diffusion flux, the compatibility equation for the equivalence factors for each region is reached:

Compatibility equation for the equivalence factors per region:

$$
\begin{equation*}
\sum_{j} V_{j} \frac{\Phi_{j, t}^{g}}{\mu_{j}^{k}}=\sum_{j} V_{j} \Phi_{j, t}^{g} \tag{14.14}
\end{equation*}
$$

We see that conservation of the leakage rate per average diffusion coefficient should be consistent with the conservation of the integrated flux on the geometry. This criterion cannot be satisfied if equivalence factors equal to 1 are set for some asymptotic cells since the problem would be over-constrained. To solve Eq. (14.14), the following functional (always positive) should be minimized:

$$
\begin{aligned}
f_{g}(\vec{\mu})= & {\left[\left(\sum_{j} V_{j} \Phi_{j, d}^{g}(\vec{\mu})\right) \Sigma_{d}^{g}-\sum_{j} V_{j} \Sigma_{j, t}^{g} \Phi_{j, t}^{g}\right]^{2} } \\
& +\sum_{j}\left[V_{j} \Sigma_{j, d}^{g} \Phi_{j, d}^{g}(\vec{\mu})-V_{j} \Sigma_{j, t}^{g} \Phi_{j, t}^{g}\right]^{2}
\end{aligned}
$$

Iterations are performed on $\sum_{j, d}^{g}$ until for each group $f_{g}(\vec{\mu})=0$.
Another possibility is to initialize the diffusion calculation with homogenized cross sections and the diffusion coefficient $D_{t}^{g}=1 /\left(3 \Sigma_{t r, t}^{g}\right)$, which is obtained directly from a transport calculation, and iterations are carried out using a fixedpoint algorithm:

$$
\left(\Sigma_{j, d}^{g}\right)_{n}=\left(\Sigma_{j, d}^{g}\right)_{n-1} \frac{\Sigma_{j, t}^{g} \Phi_{j, t}^{g}}{\left(\Sigma_{j, d}^{g} \Phi_{j, d}^{g}\right)_{n-1}}
$$

where $n$ is the current iteration and $n-1$ the previous one. Generally, this approach converges rapidly towards a solution that is not unique, given that no closure relation is imposed.

### 14.5 Homogenization Theory in Diffusion

### 14.5.1 Flux-Volume Homogenization

Homogenization with an imposed operator (e.g. diffusion) consists in achieving equivalence between two calculations performed with the same operator, either transport of diffusion. This is called iso-operator homogenization as opposed to trans-operator homogenization from a fine transport calculation to a coarse diffusion calculation. Usually, the fine discretization in space (micro-cells, e.g. pin-bypin calculation with $N$ cells) and energy (more than $J=200$ micro-groups) becomes coarser for an industrial calculation with a coarse mesh (for instance four cells per assembly, the number of macro-cells or macro-regions $M$ ) and a condensed energy mesh with $G=2$ macro-groups. The energy-integrated fluxes ${ }^{45}$ (in $\mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}$ ) for the fine calculation are denoted as $\Phi_{n=1, N}^{j=1, J}$, and as $\Phi_{m=1, M}^{g=1, G}$ for the industrial calculation. The condensation/homogenization rule by the flux-volume method applies the following formalism:

$$
\left\{\begin{array}{l}
V_{m}=\sum_{n \in m} V_{n} \\
V_{m} \Phi_{m}^{g} \equiv \sum_{j \in g} \sum_{n \in m} V_{n} \Phi_{n}^{j}
\end{array}\right.
$$

In these equations, the sign $\in$ means micro-cells belonging to a given macro-cell or micro-groups in a given macro-group. The conservation of reaction rates leads to the following definition of the condensed and homogenized cross sections:

Flux-volume condensation and homogenization:

$$
\begin{equation*}
V_{m} \Sigma_{m}^{g} \Phi_{m}^{g} \equiv \sum_{j \in g} \sum_{n \in m} V_{n} \Sigma_{n}^{j} \Phi_{n}^{j} \tag{14.15}
\end{equation*}
$$

The differential scattering cross sections are condensed as follows:

$$
V_{m} \Sigma_{m}^{g^{\prime} \rightarrow g} \Phi_{m}^{g^{\prime}} \equiv \sum_{j \in g} \sum_{j^{\prime} \in g^{\prime}} \sum_{n \in m} V_{n} \Sigma_{n}^{j^{\prime} \rightarrow j} \Phi_{n}^{i^{\prime}}
$$

The leakage cross section $\Sigma_{\text {leakage }, m}^{g} \equiv D_{m}^{g} B^{2}$ is obtained as follows:

[^312]$$
V_{m} \Sigma_{\text {leakage }, m}^{g} \Phi_{m}^{g} \equiv V_{m} D_{m}^{g} B^{2} \Phi_{m}^{g} \equiv \sum_{j \in g} \sum_{n \in m} V_{n} D_{n}^{j} B^{2} \Phi_{n}^{j}
$$

The average fission spectrum is obtained as follows:

$$
\chi_{m}^{g} V_{m} \sum_{g=1}^{G} v \Sigma_{m}^{g} \Phi_{m}^{g} \equiv \sum_{j \in g} \sum_{n \in m} \chi_{n}^{j} V_{n} \nu \Sigma_{n}^{j} \Phi_{n}^{j}
$$

where $\chi_{n}^{j}$ is the spectrum of micro-group $j$ in micro-cell $n$ averaged over the set of fissile isotopes. By construction, the neutron balance per macro-cell satisfies the following:

$$
\begin{aligned}
-\operatorname{div}\left(D_{m}^{g} \overrightarrow{\operatorname{grad}} \Phi_{m}^{g}\right)+\Sigma_{a, m}^{g} \Phi_{m}^{g} & =\left(\Sigma_{\text {leakage }, m}^{g}+\Sigma_{a, m}^{g}\right) \Phi_{m}^{g} \\
& =\sum_{g^{\prime}=1}^{G} \Sigma_{m}^{g^{\prime} \rightarrow g} \Phi_{m}^{g^{\prime}}+\frac{\chi_{m}^{g} \sum_{g^{\prime}=1}^{G} v \Sigma_{f, m}^{g^{\prime}} \Phi_{m}^{g^{\prime}}}{k_{e f f}}
\end{aligned}
$$

For two energy groups with thermal cut-off at 0.625 eV , for any macro-cell, $\chi_{m}^{1}=1$ and $\chi_{m}^{2}=0$.

### 14.5.2 Homogenization of Heterogeneous Neutron Quantities

In the previous section, "same-operator" homogenization was described such that a problem with a fine geometry (e.g. a core modeled in pin-by-pin diffusion) is made equivalent to a coarser geometry (diffusion at assembly level). In rare cases, heterogeneous diffusion to homogeneous diffusion can be justified mathematically: e.g. the case of a regular lattice of identical assemblies, or any 2D geometry with a periodic lattice. Some authors have investigated this particular problem (Planchard 1995) and F. Malige. ${ }^{46}$ The fundamental idea is based on the numerical flux distribution in periodic lattices: the flux $\Phi(\vec{r})$ has a regular structure which can be factorized as a macroscopic flux $\psi(\vec{r})$ that varies slowly at the reactor level and a microscopic flux $\varphi(\vec{r})$ that has fast variations at the level of the periodic geometry (Fig. 14.23):

[^313]

Fig. 14.23 Factorization of flux and fine structure of thermal flux [the fast flux is "out of phase" with the thermal flux, i.e. more significant in fuel than in water, (El-Wakil 1962, p. 121)]. It should be noted that power has the same distribution as thermal flux, which is even more marked since it is practically zero in water and is almost completely located within the fuel pin

$$
\begin{equation*}
\text { Flux factorization: } \quad \Phi(\vec{r})=\varphi(\vec{r}) \psi(\vec{r}) \tag{14.16}
\end{equation*}
$$

This hypothesis can be extended in a multi-group approximation regardless of the theory applied. If inserted in the one-group diffusion equation to simplify the approach, the following equation is obtained:

$$
\left\{\begin{array}{l}
-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi)+\Sigma_{t} \Phi=\frac{v \Sigma_{f} \Phi}{k_{e f f}} \text { on the reactor volume } V \\
\Phi=0 \quad \text { on the boundary } \Gamma=\partial V
\end{array}\right.
$$

The flux is assumed to be zero on the boundaries of the reactor. For each assembly $V_{i j}$ in the core computed using the infinite lattice hypothesis (i.e. the macroscopic structure is equal to one if the flux is appropriately normalized):

$$
\left\{\begin{array}{l}
-\operatorname{div}\left(D \overrightarrow{\operatorname{grad}} \varphi_{i j}\right)+\Sigma_{t} \varphi_{i j}=\frac{v \Sigma_{f} \varphi_{i j}}{k_{e f f}^{\infty}, i j} \text { on the volume } V_{i j} \text { of the assembly } \\
\frac{\partial \varphi_{i j}}{\partial \vec{n}}=0 \quad \text { on the boundary } \Gamma_{i j}=\partial V_{i j}
\end{array}\right.
$$

Using flux factorization and grouping together the terms related to the macroscopic flux, the following equation is obtained:

$$
\begin{aligned}
-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi)+\Sigma_{t} \Phi=\frac{\nu \Sigma_{f} \Phi}{k_{e f f}}= & -\varphi \operatorname{div}(\overrightarrow{\operatorname{grad}} \psi)-2 D \overrightarrow{\operatorname{grad}} \varphi \cdot \overrightarrow{\operatorname{grad}} \psi \\
& +\psi\left(-\operatorname{div}(\overrightarrow{\operatorname{Drad}} \varphi)+\Sigma_{t} \varphi\right)
\end{aligned}
$$

Since $\psi\left(-\operatorname{div}(\operatorname{Drad} \varphi)+\Sigma_{t} \varphi\right)=\psi \frac{v \Sigma_{f} \varphi_{i j}}{k_{e f f, i, j}^{\infty}}$, we finally obtain:

$$
-\varphi \operatorname{div}(D \overrightarrow{\operatorname{grad}} \psi)-2 D \overrightarrow{\operatorname{grad}} \varphi \cdot \operatorname{grad} \psi=\left(\frac{1}{k_{e f f}}-\frac{1}{k_{e f f, i, j}^{\infty}}\right) v \Sigma_{f} \varphi \psi
$$

This equation may be multiplied by $\varphi$ and simplified to:

$$
-\operatorname{div}\left(D \varphi^{2} \overrightarrow{\operatorname{grad}} \psi\right)=\left(\frac{1}{k_{e f f}}-\frac{1}{k_{e f f, i, j}^{\infty}}\right) v \Sigma_{f} \varphi^{2} \psi
$$

It may be seen that this equation in $\psi$ is always a diffusion equation, but with non-constant coefficients due to the presence of $\varphi^{2}$ (even for the piecewise equation, as was the case for the initial equation with constant coefficients per assembly). François Malige showed that in the case of a periodic lattice of the same square geometry of size $Y$, there exists a method to homogenize the coefficient $D \varphi^{2}$ of the previous diffusion equation by seeking a periodic function $\chi$ on geometry $Y$ (the assembly or a fraction of the assembly) and satisfies (by denoting $y_{1}$ the translation axis of the geometry):

$$
\overline{D \varphi^{2}}=\frac{1}{Y} \int_{Y} D \varphi^{2}(y)\left(1-\frac{\partial \chi}{\partial y_{1}}\right) d y \quad \text { with: } \quad-\operatorname{div}\left(D \varphi^{2}(y) \overrightarrow{\operatorname{grad}}\left(y_{1}-\chi\right)\right)=0
$$

Inserting this second condition in the first gives the following equation:

$$
\overline{D \varphi^{2}}=\frac{1}{Y} \int_{Y} D \varphi^{2}(y)\left(1-|\overrightarrow{\operatorname{grad} \chi}|^{2}\right) d y
$$

Calculation of $\chi$ requires the resolution of a problem with non-homogeneous boundaries where $\chi(+Y / 2)=\chi(-Y / 2)=0$ on the right and left sides and $\partial \chi(+Y / 2) /$ $\partial n=\partial \chi(+Y / 2) / \partial n=0$ on the top and bottom sides.

### 14.5.3 Average Flux Homogenization at the Boundary, Selengut Normalization

For each assembly, the microscopic flux is strictly positive when the macroscopic flux is zero at the boundaries of the reactor. The flux and current continuity between each assembly is written as:

$$
\left\{\begin{array}{l}
\Phi_{i, j}=(\varphi \psi)_{i, j}=\Phi_{i \pm 1, j \pm 1}=(\varphi \psi)_{i \pm 1, j \pm 1} \\
D_{i, j} \varphi_{i, j}\left(\frac{\partial \psi}{\partial n}\right)_{i, j}=D_{i \pm 1, j \pm 1} \varphi_{i \pm 1, j \pm 1}\left(\frac{\partial \psi}{\partial n}\right)_{i \pm 1, j \pm 1}
\end{array} \quad \text { on } \Gamma_{\cap}=\Gamma_{i, j} \cap \Gamma_{i \pm 1, j \pm 1}\right.
$$

In two-energy group theory, the approach is identical. With the same operations as those for the one-group case, the following equations result:

$$
\left\{\begin{array}{l}
-\operatorname{div}\left(D_{1} \varphi_{1}^{2} \overrightarrow{g r a d} \psi_{1}\right)+\frac{1}{k_{e f f, i, j}^{\infty}}\left(v \Sigma_{f, 1} \varphi_{1}^{2}+v \Sigma_{f, 2} \varphi_{1} \varphi_{2}\right) \psi_{1} \\
=\frac{1}{k_{e f f}}\left(v \Sigma_{f, 1} \varphi_{1}^{2} \psi_{1}+v \Sigma_{f, 1} \varphi_{1} \varphi_{2} \psi_{2}\right) \\
-\operatorname{div}\left(D_{2} \varphi_{2}^{2} \overrightarrow{g r a d} \psi_{2}\right)+\Sigma_{1 \rightarrow 2} \varphi_{1} \varphi_{2} \psi_{2}=\Sigma_{1 \rightarrow 2} \varphi_{1} \varphi_{2} \psi_{1}
\end{array}\right.
$$

The macroscopic fluxes satisfy the particular diffusion equations previously defined, which, when associated with the continuity conditions, lead to a problem called the transmission problem. Normally, the pin structure fluxes $\varphi$ that satisfy the diffusion equation on the assembly in an infinite lattice are known up to a multiplicative constant. Assuming that the macroscopic fluxes behave as a diffusion equation with constant coefficients $\widetilde{\Sigma}$ for each assembly (the real situation is more complex):

$$
\left\{\begin{array}{l}
-\operatorname{div}\left(\tilde{D}_{1} \overrightarrow{\operatorname{grad}} \psi_{1}\right)+\widetilde{\Sigma}_{a, 1} \psi_{1}=\frac{1}{k_{e f f}}\left(v \widetilde{\Sigma}_{f, 1} \psi_{1}+v \widetilde{\Sigma}_{f, 2} \psi_{2}\right) \\
-\operatorname{div}\left(\tilde{D}_{1} \overrightarrow{\operatorname{grad}} \psi_{1}\right)+\widetilde{\Sigma}_{a, 2} \psi_{2}=\widetilde{\Sigma}_{1 \rightarrow 2} \psi_{1} \\
\frac{\partial \psi_{g}}{\partial n}+\lambda_{g} \psi_{g}=0 \quad \text { on } \quad \Gamma
\end{array}\right.
$$

The flux continuity at the interfaces requires that the pin structures equal to the mean flux at the assembly boundary so as to verify the transmission conditions for the macroscopic flux on average. This is equivalent to normalizing the eigenvectors $\varphi_{g}^{0}$, which are solutions to the diffusion equation for the fine structure, by an average value at the assembly boundary:


The average homogenized cross sections (for any reaction type) used in the macroscopic diffusion problem are defined such that the reaction rate in the geometry in an infinite lattice is conserved. Hence the reaction rates computed with microscopic flux in fundamental mode are expressed as:

$$
\overline{\Sigma_{g}}=\frac{\frac{1}{S} \int_{S} \Sigma_{g} \varphi_{g}^{0} d S}{\overline{\varphi_{g}^{0}}} \quad \text { with: } \overline{\varphi_{g}^{0}}=\frac{1}{S} \int_{S} \varphi_{g}^{0} d S \quad \text { where } S \text { is the assembly surface }
$$

The homogenized quantities satisfy the normalization of the microscopic flux and are expressed as:

Average flux normalization at the boundary:

$$
\begin{equation*}
\widetilde{\Sigma}_{g}=\frac{1}{S} \int_{S} \Sigma_{g} \varphi_{g} d S=\frac{\overline{\varphi_{g}^{0}}}{\overline{\varphi_{g, \text { boundary }}^{0}}} \overline{\Sigma_{g}} \tag{14.17}
\end{equation*}
$$

This normalization of cross sections is commonly called the average flux to boundary flux normalization or the Selengut normalization. It conserves the reaction rates of the microscopic diffusion equation, and thus the infinite multiplication factor $k_{e f f, i, j}^{\infty}$ of the assembly. For the diffusion coefficient, the average transport cross section is used:

$$
\overline{D_{g}} \equiv \frac{1}{3 \Sigma_{t r, g}}=\frac{\overline{\varphi_{g}^{0}}}{\bar{S} \int_{S} \Sigma_{t r, g} \varphi_{g}^{0} d S}=\frac{\overline{\varphi_{g}^{0}}}{\frac{1}{S} \int_{S} \frac{1}{D_{g}} \varphi_{g}^{0} d S}
$$

The homogeneous diffusion coefficient $\tilde{D}_{g}$ is defined such as the leakage cross section $\overline{D_{g}} B^{2}$ is preserved, i.e.:

$$
\tilde{D}_{g}=\overline{D_{g}} \frac{\overline{\varphi_{g}^{0}}}{\overline{\varphi_{g, \text { boundary }}^{0}}}
$$

Finally:

$$
\begin{equation*}
\text { Homogenized diffusion coefficient: } \quad \tilde{D}_{g}=\frac{S}{\int_{S} \frac{1}{D_{g}} \varphi_{g}^{0} d S} \frac{\left(\overline{\varphi_{g}^{0}}\right)^{2}}{\varphi_{g, \text { boundary }}^{0}} \tag{14.18}
\end{equation*}
$$

### 14.5.4 Pin Power Reconstruction

(Planchard 1995, p. 193)

### 14.5.4.1 Convolution with Pin Power Distribution

Since safety criteria depend on local information such as the power peaking factor (Kerkar and Paulin 2008, p. 42) and the maximum temperature in a fuel rod, it is important to set up a pin power reconstruction method. If the calculation is carried out in pin-by-pin diffusion approximation, this information is readily available. However, for a coarser diffusion spatial mesh, there are two options:

- The first solution consists in superposing a pin power distribution on the mean power as was done for the flux. The pin power distribution $\pi_{i, j}^{\infty}(\vec{r})$ is then calculated in an infinite lattice with the macroscopic power being computed on the coarse diffusion mesh:

$$
\operatorname{Pow}(\vec{r}) \approx \pi_{i, j}^{\infty}(\vec{r}) \operatorname{Pow}_{i, j}(\vec{r})
$$

The pin power distribution is determined as: $\pi_{i, j}^{\infty}(\vec{r}) \equiv \sum_{g} k \Sigma_{f, g} \varphi_{i, j}^{0}$ which is normalized to the assembly power in an infinite lattice (and not by the ratio of the mean flux to the boundary flux normalization, which would lead to pin power structures per assembly that are normalized differently). Since the homogeneous power of pin k in assembly ( $\mathrm{i}, \mathrm{j}$ ) (with Nc pins releasing power ${ }^{47}$ ), is equal to $\operatorname{Pow}_{i, j}(k) \equiv \sum_{g} \overline{\kappa \Sigma_{f, g}} \psi_{g}(k)$, the factorized power is:

$$
\operatorname{Pow}(k)=\frac{\pi_{i, j}^{\infty}(\vec{r}) \text { Pow }_{i, j}(k)}{\sum_{k=1}^{N_{c}} \pi_{i, j}^{\infty}(\vec{r}) \text { Pow }_{i, j}(k)} \overline{\text { Pow }_{i, j}} \quad \text { with: } \quad \overline{\text { Pow }_{i, j}} \equiv \sum_{g} \overline{\kappa \Sigma_{f, g}} \overline{\psi_{g}}
$$

Such a formula ensures that the sum of pin powers of an assembly is equal to the mean power on the assembly. This approach leads to very small errors of less than $1 \%$ for cores constituted of UOX assemblies.

- The second solution consists in choosing the pin flux distribution for each group, then reconstructing the flux in each pin before computing the power as the following sum:

[^314]$$
\operatorname{Pow}(k)=\sum_{g} \kappa \Sigma_{f, g} \Phi(k)=\sum_{g} \kappa \Sigma_{f, g} \varphi(k) \psi(k)
$$

This is called flux factorization. Such an approach improves the precision of the calculation. For cores with various assembly types (UOX/MOX), the use of MOX distribution computed in an infinite medium has revealed the limitations of the factorization technique since a MOX is never surrounded by MOX assemblies in the core. Thus, the discrepancies increased to 5\% (a detrimental situation since the position of the peaking factor is always located in the MOX assembly). Using an infinite geometry environment when computing the pin distribution in the MOX assembly, with two or three supplementary rows of UOX pins to have more consistent solutions, reduced the discrepancy. The chief difficulty is the fact that when designing a fuel-loading pattern, the true environment of the MOX assembly is never known in advance.

### 14.5.4.2 Perturbation Approach: Rahnema Method



Farzad Rahnema(Courtesy Rahnema)
F. Rahnema ${ }^{48}$ proposed ${ }^{49,50}$ an interesting perturbation approach by expanding the power with respect to a parameter that is infinitely small compared to the current-toflux ratio at the assembly (or cell) interface. The local normalized power at position $\overrightarrow{r_{0}}$ is given by:

[^315]Pin power structure:

$$
\begin{equation*}
\pi\left(\overrightarrow{r_{0}}\right) \equiv \frac{\int_{V} d \vec{r} \int_{E=0}^{E=\infty} \kappa \Sigma_{f}(\vec{r}, E) \Phi(\vec{r}, E) \delta\left(\vec{r}-\overrightarrow{r_{0}}\right) d E}{\int_{V} d \vec{r} \int_{E=0}^{E=\infty} \kappa \Sigma_{f}(\vec{r}, E) \Phi(\vec{r}, E) d E} \tag{14.19}
\end{equation*}
$$

In this expression, $\Phi(\vec{r}, E)$ is the flux that satisfies the exact equation for the operator in a real geometry, i.e. for diffusion:

$$
\begin{aligned}
& {[K-\lambda P][\Phi(\vec{r}, E)]=} \\
& -\operatorname{div}(D(\vec{r}, E) \overrightarrow{\operatorname{grad}} \Phi(\vec{r}, E))+\left(\Sigma_{a}(\vec{r}, E)-\lambda \chi(E) v \Sigma_{f}(\vec{r}, E)\right) \Phi(\vec{r}, E) \\
& \quad-\int_{E^{\prime}} \sum_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(E^{\prime}\right) d E^{\prime}=0
\end{aligned}
$$

The quantity $\lambda$ is the largest eigenvalue of the operator $P^{-1} K[]$, usually $1 / k_{\text {eff }}$. Robin boundary conditions are expressed by introducing the infinitely small $\varepsilon$ :

$$
D(\vec{r}, E) \frac{\partial \Phi}{\partial n}+\varepsilon \gamma(\vec{r}, E) \Phi=0 \quad \text { on } \quad \Gamma=\partial V
$$

Power and flux can be expanded according to this infinitesimal quantity:

$$
\left\{\begin{array}{c}
\pi=\pi_{0}+\varepsilon \pi_{1}+O\left(\varepsilon^{2}\right) \\
\Phi=\Phi_{0}+\varepsilon \Phi_{1}+O\left(\varepsilon^{2}\right)
\end{array}\right.
$$

The values indexed by ${ }_{0}$ correspond to the non-perturbed situation, i.e. the infinite lattice case:

$$
\left[K-\lambda_{0} P\right]\left[\Phi_{0}(\vec{r}, E)\right]=0 \quad \frac{\partial \Phi_{0}}{\partial n}=0 \quad \text { on } \quad \Gamma
$$

Using the expansion of the flux and power into Taylor series in Eq. 14.19:

$$
\begin{aligned}
& {\left[\pi\left(\overrightarrow{r_{0}}\right)+\varepsilon \pi\left(\overrightarrow{r_{0}}\right)\right] \cdot \int_{V} d \vec{r} \int_{E=0}^{E=\infty} \kappa \Sigma_{f}(\vec{r}, E)\left[\Phi_{0}(\vec{r}, E)+\varepsilon \Phi_{1}(\vec{r}, E)\right] d E} \\
& \quad=\int_{V} d \vec{r} \int_{E=0}^{E=\infty} \kappa \Sigma_{f}(\vec{r}, E)\left[\Phi_{0}(\vec{r}, E)+\varepsilon \Phi_{1}(\vec{r}, E)\right] \delta\left(\vec{r}-\overrightarrow{r_{0}}\right) d E
\end{aligned}
$$

By equating the coefficient of $\varepsilon$ in a first-order expansion:

$$
\pi_{1}\left(\overrightarrow{r_{0}}\right)=\frac{\int_{V} d \vec{r} \int_{E=0}^{\infty}\left[\kappa \Sigma_{f}(\vec{r}, E)-\pi_{0}\left(\overrightarrow{r_{0}}\right)\right] \Phi_{1}(\vec{r}, E) \delta\left(\vec{r}-\overrightarrow{r_{0}}\right) d E}{\int_{V} d \vec{r} \int_{E=0}^{\infty} \kappa \Sigma_{f}(\vec{r}, E) \Phi_{0}(\vec{r}, E) d E}
$$

The perturbation of flux $\Phi_{1}$ satisfies the non-homogeneous equation:

$$
\begin{aligned}
{\left[K-\left(\lambda_{0}+\delta \lambda\right) P\right]\left[\Phi_{0}(\vec{r}, E)+\varepsilon \Phi_{1}(\vec{r}, E)\right] \approx } & \underbrace{\left[K-\lambda_{0} P\right]\left[\Phi_{0}(\vec{r}, E)\right]}_{0} \\
& +\left[K-\left(\lambda_{0}+\delta \lambda\right) P\right]_{\varepsilon} \Phi_{1}(\vec{r}, E)=0
\end{aligned}
$$

i.e.: $\left[K-\lambda_{0} P\right]=\delta \lambda P \Phi_{1}(\vec{r}, E) \quad$ with $\quad D=\frac{\partial \Phi_{1}}{\partial n}=-\gamma \Phi_{0} \quad$ on $\quad \Gamma$

This equation is multiplied by the adjoint flux $\Phi_{0}^{*}\left(\vec{r}, \overrightarrow{r_{0}}, E\right)$ of the non-perturbed situation, verifying the adjoint equation of the same eigenvalue and adjoint source $\kappa \sum_{f}(\vec{r}, E)-\pi_{0}\left(\overrightarrow{r_{0}}\right)$ in the expression of $\pi_{1}\left(\overrightarrow{r_{0}}\right)$ :

$$
\left[K^{*}-\lambda_{0} P^{*}\right] \Phi_{0}^{*}\left(\vec{r}, \overrightarrow{r_{0}}, E\right)=\kappa \Sigma_{f}(\vec{r}, E)-\pi_{0}\left(\overrightarrow{r_{0}}\right) \quad \frac{\partial \Phi_{0}^{*}}{\partial n}=0 \quad \text { on } \quad \Gamma
$$

which is integrated on the volume of the reactor and the energy spectrum. Using the Ostrogradski theorem $\left(\int_{V} \operatorname{div} \vec{f} d V=\int_{T} \vec{f} \cdot \vec{n} d S\right)$, replacing the volume integral by a surface integral and inserting the equation for the current finally leads to:

$$
\pi_{1}\left(\overrightarrow{r_{0}}\right)=\frac{\int_{\Gamma} d S \int_{E=0}^{\infty} \gamma(\vec{r}, E) \Phi_{0}(\vec{r}, E) \Phi_{0}^{*}\left(\vec{r}, \overrightarrow{r_{0}}, E\right) d E}{\int_{V} d \vec{r} \int_{E=0}^{\infty} \kappa \Sigma_{f}(\vec{r}, E) \Phi_{0}(\vec{r}, E) d E}
$$

An orthogonality condition is chosen such that the adjoint flux is unique, i.e.:
Orthogonality condition: $\int_{V} d V \int_{E=0}^{\infty} \kappa \Sigma_{f}(\vec{r}, E) \Phi_{0}(\vec{r}, E) \Phi_{0}^{*}\left(\vec{r}, \overrightarrow{r_{0}}, E\right) d E \equiv 0$

The adjoint flux exists only if:

$$
\int_{V} d V \int_{E=0}^{\infty} \Phi_{0}(\vec{r}, E)\left[\kappa \Sigma_{f}(\vec{r}, E)-\pi_{0}\left(\overrightarrow{r_{0}}\right)\right] d E=0
$$

which is true by the very definition of $\pi_{0}\left(\overrightarrow{r_{0}}\right)$ (Eq. 14.19).

Fig. 14.24 Rahnema's problem for a multiplying slab


To illustrate the method, Rahnema uses the case of slab reactor with one energy group such that there are reflective boundary conditions on the left, and a Robin condition on the right that satisfies a small $\varepsilon$. The flux of a slab reactor in an infinite medium without leakage is constant. The flux, perturbed by leakage at $x=1$, satisfies (Fig. 14.24):

$$
\Delta \Phi(x)=B_{m}^{2} \Phi(x)=0
$$

with: $B_{m}^{2}=\frac{\lambda \nu \Sigma_{f}-\Sigma_{a}}{D}$
The boundary conditions are expressed as: $\left.\frac{d \Phi}{d x}\right|_{0}=0$ and $\left.D \frac{d \Phi}{d x}\right|_{1}+\varepsilon \gamma \Phi(1)=0$
After integration of the flux, the following equation is reached:

$$
\left\{\begin{array}{l}
\Phi(x)=\Phi_{\max } \cos (B x) \\
B \tan B=\frac{\varepsilon \gamma}{D}
\end{array}\right.
$$

The normalized power is calculated by: $\pi(x)=\frac{k \Sigma_{f} \Phi(x)}{\int_{0}^{1} \kappa \Sigma_{f} \Phi(x) d x}=\frac{B \cos (B x)}{\sin B}$
This power is expanded into Taylor series for small values of $B$, and by keeping only the terms up to $B^{2}$ and using $B \tan B \approx B^{2}=\varepsilon \gamma / D$, the perturbation of the pin power distribution $\pi_{1}(x)$ (the non-perturbed pin power is equal to the unit value since the non-perturbed flux is flat) is given as:

$$
\pi(x) \approx \frac{B\left(1-\frac{B^{2} x^{2}}{2}\right)}{B-\frac{B^{3}}{6}} \approx 1+\frac{B^{2}}{6}-\frac{B^{2}}{2} x^{2}=1+\underbrace{\frac{\gamma}{2 D}\left(\frac{1}{3}-x^{2}\right) \varepsilon}_{\pi_{1}(x)}
$$

The non-perturbed adjoint flux in an infinite lattice satisfies the diffusion equation for the critical reactor without leakage in an infinite medium $\left(k_{e f f}=k_{\infty}=1, \Sigma_{a}=v \Sigma_{f}\right)$ with the adjoint source $\kappa \Sigma_{f}(x)-\pi_{0}(x)$ :

$$
-D \Delta \Phi_{0}^{*}\left(x, x_{0}\right)=\kappa \Sigma_{f}\left(1-\delta\left(x-x_{0}\right)\right) \quad \text { with: }\left.\quad \frac{d \Phi_{0}^{*}}{d n}\right|_{0}=\left.\frac{d \Phi_{0}^{*}}{d n}\right|_{1}=0
$$

which is integrated by applying the orthogonality condition, giving:

$$
\left\{\begin{array}{rll}
\Phi_{0}^{*}\left(x, x_{0}\right)=\frac{\kappa \Sigma_{f}}{D}\left(\frac{x^{2}+x_{0}^{2}}{2}+\frac{1}{3}-x_{0}\right) & \text { for } & 0 \leq x \leq x_{0} \\
\Phi_{0}^{*}\left(x, x_{0}\right)=\frac{\kappa \Sigma_{f}}{D}\left(\frac{x^{2}+x_{0}^{2}}{2}+\frac{1}{3}-x\right) & \text { for } & x_{0} \leq x \leq 1
\end{array}\right.
$$

Since the non-perturbed flux is constant, using the fact that $\gamma(0)=0$ and $\gamma(1)=\gamma$, the perturbation formula obtained after integration at the boundaries is:

$$
\pi_{1}\left(x_{0}\right)=\frac{\int_{\Gamma} d S \gamma(x) \Phi_{0}(x) \Phi_{0}^{*}\left(x, x_{0}\right)}{\int_{0}^{1} \kappa \Sigma_{f} \Phi_{0}(x) d x}=\frac{\gamma \Phi_{0} \Phi^{*}\left(1, x_{0}\right)}{\Phi_{0} \int_{0}^{1} \kappa \Sigma_{f} d x}=\frac{\gamma}{2 D}\left(\frac{1}{3}-x_{0}^{2}\right)
$$

This is similar to the analytical expression that was directly computed. By setting $\kappa \Sigma_{f}$ to 1 , the flux perturbation can be determined instead of that of the power. In the expression for the power perturbation $\pi_{1}\left(x_{0}\right)$, only the term $\gamma$ depends on the heterogeneous calculation in the perturbed situation, and fluxes $\Phi_{0}(\vec{r}, E)$ and $\Phi_{0}^{*}\left(\vec{r}, \overrightarrow{r_{0}}, E\right)$ are calculated in an infinite lattice only once. Nevertheless, it should be pointed out that the adjoint flux $\Phi_{0}^{*}\left(\vec{r}, \overrightarrow{r_{0}}, E\right)$ depends on the position $\overrightarrow{r_{0}}$, and thus, in practice, for a $P W R$ assembly with 264 fuel pins, 264 adjoint calculations are required in an non-optimized case. Symmetry considerations in the assembly in an infinite lattice may be used to allow the number of calculations to be reduced.

### 14.5.5 Discontinuity Factors

In the case of a homogenization process that preserves the reaction rates for each cell as well as the mean current for each side, the average macroscopic flux per side, $\psi_{\Gamma}$, is not generally conserved (Fig. 14.25). On the other hand, the true flux is continuous.

For highly heterogeneous cores, i.e. consisting of assemblies that are very different or with interfaces where the diffusion theory has its limitations (core/ reflector), some authors have proposed that discontinuity at the interface be taken into account (Equivalence Theory of K. Koebke, Generalized Equivalence Theory of K.S. Smith). The underlying idea is to define coefficients $f_{i, j}$ that allow for the

Fig. 14.25 Context for discontinuity factors

discontinuity of the macroscopic flux while ensuring that at the interface the following is satisfied:

$$
f_{i, j} \psi_{i, j}=f_{i \pm 1, j \pm 1} \psi_{i \pm 1, j \pm 1} \quad \text { on } \quad \Gamma_{\cap}=\Gamma_{i, j} \cap \Gamma_{i \pm 1, j \pm 1}
$$

These coefficients, which depend on the energy groups, can be calculated using a set of assemblies in an infinite lattice, or the assembly for which the discontinuity factors are required is at the center. With strict considerations, there are as many sets of discontinuity factors as the number of heterogeneous cases around the core but the problem can be reduced by averaging situations that are quite similar. The discontinuity factor is given by the following equation:

$$
f_{g}^{\Gamma_{k}}=\frac{\left.\overline{\Phi_{g}^{\mathrm{hete}}}\right|_{\Gamma_{k}}}{\left.\overline{\psi_{g}^{\text {homog }}}\right|_{\Gamma_{k}}}
$$

In this equation, the fluxes are averaged for one interface $\Gamma_{k}$ or for a set comprising two adjacent sides. The discontinuity factors can also be averaged over all the interfaces (however, with loss of precision). The homogeneous flux calculation depends on the discontinuity factors, and the latter are thus determined using an iterative scheme as for an equivalence calculation. K. Koebke proposed ${ }^{51}$ an approach based on the homogenized diffusion coefficient in each direction $(x, y)$ :

[^316]$$
J_{x}^{\text {Homog }}=-\widehat{D}_{x} \frac{\partial \psi}{\partial x} \quad \text { and } \quad J_{y}^{\text {Homog }}=-\widehat{D}_{y} \frac{\partial \psi}{\partial y}
$$

The macroscopic diffusion equation is solved by substituting the usual diffusion coefficient by the diagonal matrix of diffusion coefficients ${ }^{52}$ :

$$
\overline{\bar{D}}=\left[\begin{array}{cc}
\widehat{D}_{x} & 0 \\
0 & \widehat{D}_{y}
\end{array}\right]
$$

The leakage term is thus expressed as: $-\operatorname{div}(\overline{\bar{D}} \times \overrightarrow{\operatorname{grad}} \psi)=-\operatorname{div}\left(\widehat{D}_{x} \partial \psi / \partial x+\right.$ $\left.\widehat{D}_{y} \partial \psi / \partial y\right)$. Iterations are performed for the directional diffusion coefficients until that for a given pair $\left(K^{+}, K^{-}\right)$of opposite sides in the geometry (East, West) or (North, South), the ratios of heterogeneous flux to macroscopic flux are equal:

$$
\frac{\Phi_{K^{+}}^{\text {Hete }}}{\psi_{K^{+}}^{\text {Hog }}}=\frac{\Phi_{K^{-}}^{\text {Hete }}}{\psi_{K^{-}}^{\text {Hog }}}
$$

The same reasoning is applied for each energy group. At convergence, the directional discontinuity factor obtained is:

$$
f_{K}=\frac{\Phi_{K}^{\text {Hete }}}{\psi_{K}^{\text {Homog }}}
$$

[^317]
## Chapter 15 <br> Fuel Cycle Physics

Fuel undergoes significant nuclear transformations during its life in the reactor. Fission reactions modify isotopic concentrations and considerably affect neutron flux calculations. Heavy isotopes undergo fission and produce absorbing fission products that modify the neutron spectrum. Furthermore, fissile plutonium isotopes are also formed by capture reactions for uranium 238 and thus partially regenerate the fuel. The variations in the concentration of xenon 135-a powerful absorbing isotope produced by fission-lead to transient reactivity perturbations that can hinder the smooth running of the reactor for the operator: this is the so-called "iodine pit". Enrico Fermi experimentally discovered the "xenon effect" which may prevent the reactor from starting, although for a short period only. In the higher power Hanford reactor (USA), initially conceived to produce plutonium for the atomic bomb, Eugen Wigner allowed for voided channels as he anticipated the need to insert supplementary uranium pins to counter the xenon effect.

### 15.1 Schematic Notation for Fuel Cycle Physics

Nuclear transformations occurring in fuel (also called fuel evolution) can be studied through the use of capture/disintegration schemes. A graphical convention is adopted for the shift of the mass number by one, i.e. chemical elements are ordered by increasing atomic number $Z$, yet the shift is one unit to the left for the mass number of isotopes of a given chemical element with respect to the previous one. This notation is due to the fact that in nuclear reactors, capture reactions are predominant (naturally with fission), and thus heavier elements tend to be formed. It would therefore be difficult to view the capture scheme graphically if isotopes of the same mass were placed one above another simply because of the lack of room on the sheet of paper!

Fig. 15.1 Major disintegrations in a nuclear reactor


### 15.2 Disintegration

Nuclear fuel initially contains radioactive elements and fission/capture reactions in the reactor lead to new radioactive isotopes such as fission products or minor actinides (Fig. 15.1).

Spontaneous fission, which is the natural decay of a heavy nucleus, must be distinguished from neutron-induced fission (reaction induced by the neutron flux).

### 15.3 Neutron-Induced Reactions

These reactions take place only under neutron flux. It should be noted that radiative capture is the major capture reaction in reactors. Some reactions $(n, \alpha)$ for light target nuclei also contribute significantly, such as the capture of ${ }_{5}^{10} B$, mentioned earlier (Fig. 15.2).

### 15.4 The Bateman Equations

From the appearance/disappearance of a nuclide, three balance equations can be expressed: one for the heavy nuclei, a second for fission products and a third for activation products, all in the form of first-order differential equations. The homogeneous form of these differential equations was studied for families of radioactive isotopes by Harry Bateman in 1910. ${ }^{1}$ In 1962, the inhomogeneous form (with a

[^318]Fig. 15.2 Major neutron capture reactions taken into account in reactors

fission term) was studied in the form of "linearized chains" by T. R. England (Stamm'ler and Abbate 1983, p. 384) for the CINDER code. Below are the most common balances (i.e. those with the most commonly encountered reactions or decays).

### 15.4.1 Heavy Nuclides

The term heavy nuclides requires clarification. Usually, they refer to isotopes with proton number larger than that of lead, which has isotopes that constitute the end of decay chains. However, according to context, they are often defined as chemical elements that cannot be produced by fission, and in more restricted cases, the transactinides (Photo 15.1).

Certain chemical elements such as gadolinium are sometimes called heavy nuclides but in this case, their proton number is used, since gadolinium can be produced by fission of a fissile nucleus.

[^319]Photo 15.1 Harry Bateman (1882-1946) (Public domain)


Let:

- $N(t)$ be the number of nuclei of a given heavy nuclide ${ }_{Z}^{A} X$ at a given time,
- $\lambda_{\beta^{+}}$(resp. $\beta^{-}, \alpha, \gamma$, spontaneous fission), the decay constant of the $\beta^{+}$decay (resp. $\beta^{-}, \alpha, \gamma$, spontaneous fission),
- $\sigma_{(n, \gamma)}$ the microscopic cross section of radiative capture (resp. $\sigma_{(n, 2 n)}$ for the reaction $(n, 2 n)$ ),
- $\Phi$ the neutron flux during depletion.

The differential equation of the balance is expressed as:

$$
\begin{aligned}
& \frac{d N(t)}{d t}\left[\begin{array}{l}
A \\
Z
\end{array}\right]=\Phi\left[\sigma_{(n, \gamma)} N(t)\right]\left[\begin{array}{c}
A-1 \\
Z
\end{array}\right] \\
& +\Phi\left[\begin{array}{ll}
\sigma_{(n, 2 n)} & N(t)
\end{array}\right]\left[\begin{array}{c}
A+1 \\
Z
\end{array}\right] \\
& +\left[\lambda_{\beta^{+}} N(t)\right]_{\left[\begin{array}{c}
A \\
Z+1
\end{array}\right]}+\left[\lambda_{\beta^{-}} N(t)\right]_{\left[\begin{array}{c}
A \\
Z-1
\end{array}\right]} \\
& +\left[\begin{array}{ll}
\lambda_{\alpha} & N(t)
\end{array}\right]\left[\begin{array}{l}
A+4 \\
Z+2
\end{array}\right]+\left[\begin{array}{ll}
\lambda_{\gamma} & N(t)
\end{array}\right]\left[\begin{array}{l}
A \text { meta } \\
Z
\end{array}\right] \\
& -\Phi\left[\left(\sigma_{\text {capture }}+\sigma_{\text {fission }}+\sigma_{(n, 2 n)}\right) \cdot N(t)\right]\left[\begin{array}{l}
A \\
z
\end{array}\right] \\
& -\left[\left(\lambda_{\beta^{-}}+\lambda_{\beta^{+}}+\lambda_{\alpha}+\lambda_{\gamma}+\lambda_{\text {spontaneous fission }}\right) N(t)\right]_{\left[\begin{array}{c}
A \\
z
\end{array}\right]}
\end{aligned}
$$

The source terms lead to an increase in $N(t)$ and have a positive sign, whereas those with a negative sign indicate the disappearance of the nuclide. In this equation, only the most common capture/decay reactions have been included. The notation:

$$
\lambda_{\text {total }}=\lambda_{\beta^{-}}+\lambda_{\beta^{+}}+\lambda_{\alpha}+\lambda_{\gamma}+\lambda_{\text {spontaneous fission }}
$$

introduces the notion of partial decay branching $B r_{i}$ (or branching ratio) for isotopes that have several decay channels. In this case, the partial decay constants are given by:

$$
\lambda_{i}=B r_{i} \lambda_{\text {total }}
$$

### 15.4.2 Fission Products

As their name indicates, fission products are created during the fission of a heavy nuclide. They are often radioactive and decay by $\beta^{-}$or $\gamma$, and seldom through $\beta^{+}$. The production term by fission is the sum of the fission rates of fissile isotopes multiplied by the fission yield of the considered isotope.

$$
\begin{aligned}
& \frac{d N(t)}{d t}\left[\begin{array}{l}
A \\
Z
\end{array}\right]=\Phi\left[\begin{array}{ll}
\sigma_{(n, \gamma)} & N(t)]_{\left[\begin{array}{c}
A-1 \\
Z
\end{array}\right]}+\left[\lambda_{\beta^{+}} N(t)\right]_{\left[\begin{array}{c}
A \\
Z+1
\end{array}\right]} .{ } . \\
\end{array}\right. \\
& +\left[\lambda_{\beta^{-}} N(t)\right]_{\left[\begin{array}{c}
A \\
Z-1
\end{array}\right]}+\left[\begin{array}{ll}
\lambda_{\alpha} & N(t)
\end{array}\right]\left[\begin{array}{c}
A+4 \\
Z+2
\end{array}\right]+\left[\lambda_{\gamma} N(t)\right]_{\left[\begin{array}{c}
\text { A meta } \\
Z
\end{array}\right]} \\
& -\Phi\left[\sigma_{(n, \gamma)} N(t)\right]_{\left[\begin{array}{l}
A \\
Z
\end{array}\right]}-\left[\left(\lambda_{\beta^{-}}+\lambda_{\beta^{+}}+\lambda_{\alpha}+\lambda_{\gamma}\right) \cdot N(t)\right]_{\left[\begin{array}{c}
A \\
Z
\end{array}\right]+Y_{G}\left[\begin{array}{c}
A \\
Z
\end{array}\right] . ~}^{\text {Z }}
\end{aligned}
$$

$Y_{G}\left[\begin{array}{l}A \\ Z\end{array}\right]$ is the global fission yield of isotope ${ }_{Z}^{A} X$, i.e.:

$$
Y_{G}\left[\begin{array}{l}
A \\
Z
\end{array}\right]=\sum_{\text {All fissile nuclei } \mathrm{F}} \gamma_{\left[\begin{array}{c}
A \\
Z
\end{array}\right]^{\tau} \tau_{F} .}
$$

with: $\tau_{F}$ the fission rate of fissile isotope $F$;
$\gamma_{\left[\begin{array}{l}A \\ Z\end{array}\right]}^{F}$ the fission yield of isotope ${ }_{Z}^{A} X$ from $F$.
The nuclear data libraries provide the total decay constants $\left(\lambda_{T}\right)$ and the decay branching ratios normalized to one, such that $\lambda_{i}=B r_{i} \lambda_{T}$. The first term $\Phi\left[\sigma_{(n, \gamma)} N(t)\right]$ does not allow for the capture branch since it is assumed that $\sigma_{n, \gamma}$ accounts for it (meaning that there are two different cross sections for the balance carried out for the isotope in its ground state or metastable state). Indeed, a given reaction for a particular nuclide may not exist (thus, $\sigma_{\text {reaction }}=0$ ). The same is possible for a given decay.

### 15.4.3 Activation Products

In some reactor structures (grids, rod bank mechanisms, baffle, steel parts, etc.), certain isotopes have an absorption cross section that leads to the production of new isotopes, which are often radioactive. Some emit highly penetrating rays, e.g. cobalt 60. The structure elements do not contain any fissile isotope by definition, and thus, there is no fission production in the equation for activation products, which is very similar to that of the heavy nuclides:

$$
\begin{aligned}
\frac{d N(t)}{d t}\left[\begin{array}{l}
A \\
Z
\end{array}\right]= & \Phi\left[\begin{array}{ll}
\sigma_{(n, \gamma)} & N(t)
\end{array}\right]\left[\begin{array}{c}
A-1 \\
Z
\end{array}\right]+\Phi\left[\begin{array}{l}
\sigma_{(n, 2 n)} \\
N(t)
\end{array}\right]\left[\begin{array}{c}
A+1 \\
Z
\end{array}\right] \\
& +\left[\begin{array}{ll}
\lambda_{\beta^{+}} & N(t)]\left[\begin{array}{c}
A \\
Z+1
\end{array}\right]+\left[\lambda_{\beta^{-}} N(t)\right.
\end{array}\right]\left[\begin{array}{c}
A \\
Z-1
\end{array}\right]+\left[\begin{array}{ll}
\lambda_{\gamma} & N(t)
\end{array}\right]\left[\begin{array}{c}
A \text { meta } \\
Z
\end{array}\right] \\
& -\Phi\left[\left(\sigma_{(n, \gamma)}+\sigma_{(n, 2 n)}\right) \cdot N(t)\right]\left[\begin{array}{c}
A \\
Z
\end{array}\right]-\left[\left(\lambda_{\beta^{-}}+\lambda_{\beta^{+}}+\lambda_{\gamma}\right) N(t)\right]\left[\begin{array}{c}
A \\
Z
\end{array}\right]
\end{aligned}
$$

Activation reactions are often threshold reactions or reactions such as $(\alpha, n)$ or ( $\alpha, p$ ).

### 15.4.3.1 Example of the Cobalt 60 Chain

Cobalt (from kobold: meaning mischievous spirit due to its toxic ores) was discovered in 1735. For centuries, cobalt salts have been used to obtain the blue color for enamels and porcelain. However, if employed in a steel alloy, the latter has some particular properties. In reactors, cobalt exists in the form of trace elements in the zirconium of claddings (from 0.002 to $0.15 \%$ ), in Inconel 600 (less than $0.1 \%$ ) and in stainless steel (less than $0.2 \%$ ). One of its isotopes, cobalt 60 , is radioactive and emits $\beta^{-}$particles. The main production channel is through capture on cobalt 59. Cobalt 60 emits highly penetrating $\gamma$ radiation (with an emission ray at 1.17 MeV and another at 1.33 MeV ). It thus represents a danger for radioprotection in the case of over-exposure. Cobalt radiation was in fact used in radiotherapy until the 1960s to cure certain cancers (via the destruction of target cancerous cells) by a process inaccurately referred to popularly as the "cobalt bomb" (Fig. 15.3).

The Bateman equation for cobalt 60 is written as:

$$
\text { Cobalt 60 equation: } \left.\begin{array}{rl}
\frac{d\left[{ }_{27}^{[60} \mathrm{Co}\right]}{d t}= & \Phi \sigma_{n, \gamma)}^{\left[{ }^{[27} \mathrm{Co}\right]}\left[{ }_{27}^{59} \mathrm{Co}\right]+\lambda_{T I}\left[{ }_{27}^{60 \mathrm{~m}} \mathrm{Co}\right] \\
& \left.-\Phi \sigma_{(n, \gamma)}^{[60} \mathrm{Co}\right] \tag{15.1}
\end{array}{ }_{27}^{60} \mathrm{Co}\right]_{\left.{ }_{27}^{60} \mathrm{Co}\right]}-\lambda_{\beta^{-}}\left[{ }_{27}^{60} \mathrm{Co}\right] .
$$



Fig. 15.3 Cobalt 60 production chain

### 15.5 Vectorial Form of the Bateman Equation

For a set of nuclides that depend on one another through decay chains or other reactions, the following differential system can be expressed:

Let $\vec{N}(t)$ be the isotopic compositions vector; its components are the various concentrations of isotopes $N_{i}(t)$ :

$$
\begin{cases}\frac{d \vec{N}_{\text {heavy }}(t)}{d t}=A \vec{N}_{\text {heavy }}(t) & \text { for heavy nuclides } \\ \frac{d \vec{N}_{F P}(t)}{d t}=B \vec{N}_{F P}(t)+S & \text { for fission products } \\ \frac{d \vec{N}_{A P}(t)}{d t}=C \vec{N}_{A P}(t) & \text { for activation products }\end{cases}
$$

These differential equations are commonly known as the generalized Bateman differential equations. Usually for a pressurized water reactor based on a uranium/ plutonium cycle:

$$
\vec{N}_{\text {heavy }}=\left(\begin{array}{c}
{ }_{92}^{234} U \\
235 \\
92 \\
238 \\
92 \\
\vdots \\
244 \\
96 \\
9 m
\end{array}\right) \quad \vec{N}_{F P} \text { depends on the application }
$$

### 15.6 Calculation of Relevant Quantities for the Fuel Cycle

### 15.6.1 Mass Balance

One of the most extensively required calculations in fuel cycle is that of the fuel composition at different burn-ups. This is the mass balance application. It
corresponds to a nuclide count. The mass $M$ in grams for a nuclide in a given volume is obtained as:

$$
M=\frac{N}{\mathcal{N}} A
$$

where: $\mathcal{N}$ is the Avogadro number $\left(6.022 \times 10^{23} \mathrm{~mol}^{-1}\right)$,
$A$ is the atomic mass of the considered nuclide (in g ),
$N$ is the number of nuclides in the considered volume (in number of nuclides).
If $N$ is expressed in nuclides $/ \mathrm{cm}^{3}$, the mass is obtained in grams $/ \mathrm{cm}^{3}$.

### 15.6.2 Burn-up

Burn-up is a particularly useful quantity which characterizes the energy which has been produced by the fuel under flux. It is usually expressed as the ratio of the total energy produced (expressed for industrial reactors as MWd, i.e. MegaWatt-day, or in GWd, GigaWatt-day) to the mass in tonnes of initial heavy metals. The choice of this reference avoids the difficulty of using a reference linked to the current mass of fuel since during fission, the mass of heavy metals varies with time. This normalization also allows direct comparisons of the efficiency of several fuel management approaches for a given reactor series or by different fractioning of fuel for reloading. Knowing the burn-up in MWd/t enables direct evaluation of energy by multiplying the specific power per unit mass by the number of operating days.

### 15.6.2.1 Thermal Burn-up

Burn-up characterizes the amount of energy produced by a nuclear fuel. Rather than the unit Joule/kg, engineers use an International system unit that allows rapid calculation of the energy delivered by a nuclear reactor: the MegaWatt-day per metric tonne (MWd/t).

$$
\text { Thermal burnup }{ }_{[M W d / t]} \equiv \frac{\text { Released energy }_{[M W d]}}{\text { Initial mass of heavy metal } \operatorname{man}_{[t]}} .
$$

It should be pointed out that only the mass of the fissile fuel (metal) is counted and not the total mass of the oxide $U O_{2}$ in the case of $U O_{2}-P W R$. Thus, the oxygen atoms in the oxide are not included. In thermal neutron reactors, the term thermal burn-up is employed:

$$
\text { Thermal burn - up: } T C T \equiv \frac{\left(\sum_{\sum_{\text {fissile nuclei }} \kappa_{f} N_{f}} \sigma_{f}\right.}{} \begin{align*}
& )_{[M W]}  \tag{15.2}\\
& \text { fuel mass }_{[t]}
\end{align*} \Delta t_{[d]} \quad \text { in } M W d / t
$$

with: $k_{f} \approx 200 \mathrm{MeV} /$ fission $\times 1.6 \times 10^{-19} \mathrm{~J} / \mathrm{eV}=3.2 \times 10^{-17} \mathrm{MJ} /$ fission
$N_{f}$ concentration of a fissile nuclide in [nuclides in the considered mass]
$\sigma_{f} \Phi$ microscopic fission rate in [fissions/s]
$\Delta t$ time increment in operating days [days]
If concentrations are expressed per metric tonne, the fuel mass is taken as equal to 1 ton, otherwise the mass corresponding to the considered volume is used. Thermal burn-up corresponds to the product of the Specific Thermal Power of the reactor multiplied by the number of operating days at that power:

$$
T B U=P_{\text {specific }}[M W / t] \Delta t_{[d]}
$$

For a 900 MWe $E D F$ reactor with a third-core fuel management (initial enrichment for ${ }_{92}^{235} U$ is $3.25 \%$ ), the unloading burn-up is $33,000 \mathrm{MWd} / \mathrm{t}$. For a quarter-core fuel management, (initial enrichment for ${ }_{92}^{235} U$ is $3.70 \%$ ), it is $42,000 \mathrm{MWd} / \mathrm{t}$. The initial mass of heavy metal (which only includes uranium, and at most plutonium and americium 241 for MOX fuel) must not be confused with a tonne of initial oxide such as $\mathrm{UO}_{2}$ or $\mathrm{PuO}_{2}$, or even a tonne of heavy metal at the current burn-up. The mass of heavy nuclides decreases significantly by fission, thereby creating fission products. The main difficulty resides in the following formulation of the total power produced:

Power calculation: Power $_{[M W]}=\sum_{\text {Fissile nuclides }} \kappa_{f} \sigma_{f} N_{f} \Phi+\sum_{\text {Capturing nuclides }} \kappa_{c} \sigma_{c} N_{c} \Phi$

Thus, the quantity $\kappa_{f}$, which represents the total energy released by a neutron inducing fission, must be defined. Nevertheless, the question arises of how to account for the energy dissipated in water (either by the slowing down of neutrons or by attenuation-analogous to "friction"-of $\gamma$ rays in water) and in structural elements (with the same physical phenomena). The thermal power released by the fuel pin of a water reactor can be broken down into:

$$
P_{\text {fuel }}=P_{\text {recoil }+\beta}+P_{\gamma \text { autoabsorption }}+P_{\gamma \text { from neighboring pins }}
$$

where: $P_{\text {recoil }+\beta}$ is the thermal power released in the fuel pin, i.e. the energy (per unit time) of recoil of fission products that are stopped locally and the energy of $\beta$ particles that are also absorbed on the spot.
$P_{\gamma \text { autoabsorption }}$ is the power absorbed in the pin (called auto-absorption), where the $\gamma$ particles were emitted either by fission (prompt or delayed $\gamma$ ) or by capture of the $\nu-1$ other neutrons released by fission (one neutron induces fission, the others are mainly captured by $(n, \gamma)$ reactions or leak out from the reactor-in small amounts). The $\gamma$ produced lose their energy in the reactor.
$P_{\gamma \text { from neighboring pins }}$ is the power obtained from the $\gamma$ rays originating from the neighboring pins which are formed by the same mechanisms as above.

This is the power that is released in the fuel, and it must be added to that released in the inactive structures of the core:

$$
P_{\text {geometry }}=P_{\text {fuel }}+P_{\gamma \text { water }+ \text { structure }}+P_{\text {neutron }} \quad \text { slow-down }
$$

with: $P_{\gamma \text { water }+ \text { structure }}$ is the power deposited in the water by $\gamma$ rays and in the structures by $\gamma$ stemming from radiative capture by the $\nu-1$ other neutrons released by fission, as well as the $\gamma$ from fission emanating from the fuel. The contribution of massive structures such as cladding and grids is significant compared to that of water.
$P_{\text {neutron }}$ slow-down is the power of neutrons that are mainly slowed down in water and release 2 MeV per neutron as kinetic energy on slowing down from the mean energy of a Watt spectrum ( 2 MeV ) to thermal energy ( $1 / 40 \mathrm{eV}$, i.e. almost $0 \mathrm{MeV})$. Since $\nu$ neutrons are produced $(\approx 2.5)$, this energy is about 5 MeV per fission.

Numerical simulations (Monte Carlo calculations) for the deposited energy in the structures and water showed that the power deposited outside the fuel is around: ${ }^{2}$

$$
P_{\gamma \text { water }+ \text { structure }}+P_{\text {neutron }} \quad \text { slow-down } \approx 2.6 \%
$$

This power is injected directly into water in core thermal-hydraulic calculations, especially if there is no need to locate the power in the cladding or in the fuel. It is common practice to attribute to the fission energy, $\kappa_{f}$ (Table 15.1), the total energy that can be obtained from fission of the atom, i.e. the recoil energy of fission products (about 166 MeV ), the energy of prompt $\gamma$ (about 8 MeV ), the energy of delayed $\gamma$ (about 7 MeV ), the energy of $\beta$ particles (about 7 MeV ), and the kinetic energy of $\nu$ neutrons (about 5 MeV ). The energy of neutrinos is lost. The energy produced by the capture of $\nu-1$ neutrons that do not induce any fission is not included in this energy balance.

The capture energy (Table 15.2), weighted by the capture rate, must be added to the fission power by summation of the capturing isotopes in the geometry (and not only those in the fuel since power is also released in non-fissile zones). For

[^320]Table 15.1 Mean fission energy $(\mathrm{MeV})$ for the main fissile isotopes

|  | ${ }_{92}^{235} U$ | ${ }_{92}^{236} U$ | ${ }_{92}^{238} U$ | ${ }_{94}^{238} P u$ | ${ }_{94}^{239} P u$ | ${ }_{94}^{240} \mathrm{Pu}$ | ${ }_{94}^{241} \mathrm{Pu}$ | ${ }_{94}^{242} P u$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $\kappa_{f}$ | 193.1 | 194.5 | 193.8 | 197.4 | 198.5 | 199.5 | 202.5 | 201.6 |

simplified calculations where parasite captures are not disregarded, a mean value of 6 MeV may be added for each supplementary radiative capture, i.e. around $(\nu-1)$ $6 \mathrm{MeV}=8 \mathrm{MeV}$ to the fission energy per isotope. Thus, the depletion flux for a fuel normalized to a specific power in $\mathrm{W} / \mathrm{g}$ may be calculated as follows:

Fluxinageometry:

$$
\begin{equation*}
\Phi_{\left[n / \mathrm{cm}^{2} / \mathrm{s}\right]}=\frac{\text { Power }_{[\mathrm{W} / \mathrm{g}]}}{\sum_{\text {Fissile nuclides }} \kappa_{f[J]} \sigma_{f\left[\mathrm{~cm}^{2}\right]} N_{f[\text { atom } / \mathrm{g}]}+\sum_{\text {Capturing nuclides }} \kappa_{c[J]} \sigma_{c\left[\left[\mathrm{~cm}^{2}\right]\right.} N_{c[\text { atom } / \mathrm{g}]}} \tag{15.4}
\end{equation*}
$$

While it is completely rational to integrate the power released by capture in the calculation of the flux level (in which case, the latter is artificially increased to compensate for the uncounted power), burn-up is a more complex matter. Indeed, if only fission power $\sum_{\text {fissiles nuclides }} \kappa_{f} \sigma_{f} N_{f} \quad \Phi$ and power from captures
$\sum \quad \kappa_{c} \sigma_{c} N_{c} \Phi s$ are accounted for in the fuel zone, the power produced in capturing nuclides
cladding and in water is neglected. This term is evaluated as being $0.5 \%$ of the total power. It should be pointed out that this amount is less than $2.6 \%$ of the power deposited in the structures mainly because of the fact that the kinetic energy of neutrons is already included in the fission energy $\kappa_{f}$. Thus, the energy does not represent the energy deposited in the fuel but rather the energy that can be obtained in a given geometry. The definition of burn-up is hence impacted. Indeed, the energy produced in the non-fissile zones cannot be used to define burn-up in these zones due to the absence of fissile mass. The only power that can in fact be measured is that delivered at the turbine, and hence, using the cycle efficiency, the total thermal power released by the reactor is obtained (e.g. 2775 MWthermal for a CPY series). After dividing by the mass of fissile metal in tonnes, this power determines the specific depletion power, which is itself used to evaluate the number of Effective Full Power Days (EFPD) by dividing burn-up by specific power. Hence, thermal burn-up does not provide a direct snapshot of the fissions solely in the fuel, but rather of the total energy delivered by the assembly.

It should be noted that thermal burn-up can be determined experimentally either by exact monitoring of a reactor, giving the number of Equivalent Full Power Days (EFPD), or by destructive measurements of fuel pins and measuring the amount of fission products that are good indicators of burn-up, such as neodymium 148.
Table 15.2 Mean capture energy $(\mathrm{MeV})$ for the major isotopes

|  | ${ }_{2}^{4} \mathrm{He}$ | ${ }_{5}^{10} \mathrm{~B}$ | ${ }_{5}^{11} \mathrm{~B}$ | ${ }_{6}^{12} \mathrm{C}$ | ${ }_{7}^{14} \mathrm{~N}$ | ${ }_{7}^{16} \mathrm{O}$ |  | ${ }_{11}^{23} \mathrm{Na}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |

### 15.6.2.2 Fission Burn-up (for Fast Neutron Reactors)

Fission burn-up is closer to actual physical phenomena, and is interesting as it locates the production of power geometrically and avoids the various difficulties discussed in the definition of thermal burn-up. Two types of fission burn-up are defined:

- \%FIFA for Fission per Invested Fissile Atom, which represents the number of fissions normalized to the number of fissile atoms:

$$
\% F I F A \equiv 100 \quad \frac{\int \Sigma_{f} \Phi d t}{N_{f}(0)} \text { in } \%, \text { where } N_{f}(0) \text { is the initial number of heavy }
$$

fissile atoms

- \%FIMA for Fission per Invested Metal Atom, which is the initial number of heavy atoms:
$\%$ FIMA $\equiv 100 \quad \frac{\int \Sigma_{f} \Phi d t}{N(0)}$ in $\%$, where $N(0)$ is the number of heavy atoms.
Fission burn-up (dimensionless) is used mainly in the case of fast neutron reactors. \%FIMA is used more widely than \%FIFA as it provides a better estimate of the initial amount of nuclides (fertile nuclides also lead to fissions). $1 \%$ FIMA corresponds to $10,000 \mathrm{MWd} / \mathrm{t}$.


### 15.6.2.3 Fuel Depletion with Burn-up

For heavy nuclides, the Bateman equation can be expressed in the simplified form:

$$
\frac{d N}{d t}=-\lambda N+\Sigma \Phi
$$

Usually, in the case of decays (mainly $\alpha$ ) of heavy nuclides during the uraniumthorium cycle, decay by radioactivity is considered negligible compared to the capture rate $(\lambda N \ll \Sigma \Phi)$, especially for the isotopes ${ }_{92}^{235} U,{ }_{92}^{238} U$ and ${ }_{94}^{239} P u$.

Hence: $\Delta N \approx \Sigma \Phi \Delta t$
The product of flux and time, $\Phi t$, is called the neutron fluence, and is often expressed in neutron/kilobarn. $\Phi \Delta t$ is thus a fluence increment. Since burn-up is proportional to the specific power level:

$$
\Delta \tau=P_{\text {specific }} \Delta t
$$

and the power itself being proportional to the flux as given by Eq. (15.4), it may be deduced that fluence is invariable to an increase in specific power when the time step is inversely proportional to this increase. Hence, a fuel that is subjected to twice a given power during a time period which is halved has undergone the same fluence, and thus the same burn-up. The concentrations of heavy nuclides of this long period thus depend at first order on burn-up and not on time. This specificity is
widely employed in the generation of cross-section libraries for reactor calculations where the cross sections depending on self-shielding, especially on the concentrations of resonant isotopes, are tabulated in terms of burn-up only and not concentrations. This approximation is justified in most cases, except that of ${ }_{94}^{241} \mathrm{Pu}$, which has a shorter period ( 14.3 years) and transforms into ${ }_{95}^{241} \mathrm{Am}$, thereby leading to an excess in absorption. This property whereby cross sections depend on burn-up only is universally employed in calculation codes for reactor physics.

### 15.6.3 Activity

Activity, i.e. the number of disintegrations per second at a given time, is computed as follows:

$$
\begin{equation*}
\text { Radioactive activity: } \quad A_{[B q]} \equiv \lambda_{\left[s^{-1}\right]} N_{[\text {atoms }]} \tag{15.5}
\end{equation*}
$$

Since 1975, the official unit of activity is the becquerel (Bq). A more suitable unit for industrial computations is the curie $=3.7 \times 10^{10} \mathrm{~Bq}$, named in honor of Pierre and Marie Curie, and which corresponds to the activity of one gram of radium 226. The activity per unit volume is obtained by dividing the activity of a given element by its volume [in $\left(\mathrm{Bq} / \mathrm{cm}^{3}\right)$ ], and the same definition is applied for the activity per unit mass [in $(\mathrm{Bq} / \mathrm{kg})]$. A stable isotope has an activity of zero.

### 15.6.4 Calculation of Decay Heat

Radioactivity is associated with energy emission. The decay heat $(D H)$ corresponds to the energy of the radioactivity emitted per unit time for a given mass of radioactive products (reactor core, radioactive waste container, stocking pool, etc.). The decay heat is of paramount importance for reactor safety since even after control rods have been inserted, a significant amount of power must still be cooled by core cooling systems even when the reactor is not operating. This power decays quickly after rod insertion and decreases slowly after 1 h to $1 \%$ of the nominal power. One year after a reactor has stopped, it is still worth $1 / 1000$ its nominal power. For engineering applications, the empirical Way-Wigner formula, established in 1948, can be applied (Baur 1985, p. 192):

$$
\begin{equation*}
\text { Way-Wigner formula: } \frac{P(t)}{P_{0}}=0.0622\left(t^{-0,2}-\left(t+t_{i r r}\right)^{-0,2}\right) \tag{15.6}
\end{equation*}
$$

where t is the time in seconds after rod insertion and $t_{i r r}$ is the operating period of the reactor in seconds. For fresh fuel, the decay heat of $\alpha$ emitters is called the inherent power. The term decay heat is used for fission products.

### 15.6.4.1 Summation Method

For each nuclide, $i$, the decay heat, DH , in watts is obtained by multiplying the activity by the energy released per disintegration:

Decay heat of anisotope: $D H_{i(\text { Watt })}=\lambda_{\left(s^{-1}\right)} N_{\text {(number of atoms of nuclide } i)}\left(\bar{E}_{\gamma}+\bar{E}_{\beta}+\bar{E}_{\alpha}\right)$

$$
\begin{equation*}
\times 1.610^{-13} \tag{15.7}
\end{equation*}
$$

where $\bar{E}_{\gamma}, \bar{E}_{\beta}$ and $\bar{E}_{\alpha}$ are the mean energies released for the radioactivity of the same name (in MeV , and the unit conversion of $1.6 \times 10^{-13}[\mathrm{~J} / \mathrm{MeV}]$ is applied), per nuclide considered. It may be seen that $\bar{E}_{\gamma}+\bar{E}_{\beta}+\bar{E}_{\alpha}$ is the energy released for any disintegration ( $\gamma, \beta$ or $\alpha$ ) through the definition of mean energy. Note that it is erroneous to suppose that an $\alpha$ decay emits only an energy corresponding to $\bar{E}_{\alpha}$. Indeed, an $\alpha$ or $\beta$ decay is also followed by a $\gamma$ decay. The total decay heat is the sum of the power released by the set of isotopes that make up the considered medium:

$$
\begin{equation*}
\text { Decay heat by summation: } \quad D H_{\text {total }}=\sum_{i} D H_{i} \tag{15.8}
\end{equation*}
$$

This calculation method, also naturally called a summation method, is exact but requires precise knowledge of the fuel composition or the core for which the decay heat is being computed. The Laugier curve ${ }^{3}$ method provides a simplified way to obtain the number of isotopes that must be accounted for with respect to a given

[^321]
(Courtesy Laugier)


Fig. 15.4 Laugier curves for short cooling times
precision for the decay heat of a given fuel (Fig. 15.4)—since a reference calculation of decay heat with a large number of isotopes is available. The more precision that is required, the greater the number of isotopes that must be taken into account. Furthermore, for different cooling times, it is not the same isotopes (unfortunately!) that require calculation. Thus, for long cooling times (geological times), only a few isotopes with a long half-life are required whereas the decay heat for very short cooling times (just after scram) requires over a hundred isotopes are needed. Nowadays, the best-estimate calculations are carried out with more than 1200 isotopes for which the energy per disintegration is known. Indeed, the disadvantage of reference codes is the long computational times involved, since at present, calculation of the isotopic composition of an assembly takes more than half an hour.

For example, for a cooling time of 22 days (Fig. 15.5, time in days on a logarithmic scale), 32 isotopes are required to capture $99 \%$ of the decay heat, and 95 are required for a precision of $99.9999 \%$. For a precision of $10^{-12} \%, 272$ isotopes are required. The hash-and-dot plot represents the cumulated number of isotopes required to obtain a given precision of the decay heat for any cooling time. This number increases during cooling to allow for the fact that new isotopes become more dominant as cooling times increase. However, the black plot at $90 \%$ shows that fewer isotopes are required between 10,000 days and 1 million days compared to 100 million days. Hence, it is difficult calculate the decay heat with codes using summation since the decay chains depend on the cooling time.


Fig. 15.5 Laugier curves for geological times

Usually, the decay heat is decomposed into three terms:

$$
D H_{\text {total }}=D H_{\text {delay }}+D H_{F P}+D H_{H N}
$$

The power of delayed neutrons $D H_{\text {delay }}$ corresponds to the fission induced by delayed neutrons. Due to the longer period of delayed neutrons ( 56.4 s ), it is assumed that their decay heat is negligible after 10 min . Nevertheless, it is the dominant term during the initial seconds following the rod insertion. This term will be discussed in the chapter on kinetics. The power due to fission products $D H_{F P}$ corresponds to the energy released due to the $\gamma$ produced by $\beta$ decay of fission products. The power due to heavy nuclides $D H_{H N}$ stems from the kinetic energy of $\alpha$ and $\gamma$ particles emitted by heavy nuclides, and seldom $\beta$ decays. Common practice separates contributions from $\beta^{-}$decays of the ${ }_{92}^{239} U \rightarrow{ }_{93}^{239} \mathrm{~Np} \rightarrow{ }_{94}^{239} P u$ decay chain, which is mainly dominant during the 20 initial cooling days from those due to $\alpha$ decays of heavy nuclides.

### 15.6.4.2 Decay Heat Burst Function

The decay heat calculation of fission products can be evaluated more quickly without determining their concentration using the Decay Heat Power Burst Function ( $D H B F$ ), which indicates the evolution of the decay heat due to fission products from one fission per heavy nuclide considered and per incident neutron energy
(thermal neutron at 0.0253 eV , fast neutron at 400 keV and fusion neutron at 14 MeV ). ${ }^{4}$

Let $[0, T]$ be the irradiation time interval and $\Delta t_{\text {cool }}$ the cooling time after irradiation. If $t$ is the time at which decay heat is being calculated with the origin being immediately after the reactor is stopped, the decay heat at time $t$ is the convolution of the DHBF for each fissile isotope $F$ by the fission rate of this isotope integrated over the irradiation time:

$$
D H_{F}(t)=\int_{0}^{T} N_{F}(\tau) \sigma_{f}^{F}(\tau) \Phi(\tau) \operatorname{DHBF}_{F}(T+t-\tau) d \tau
$$

This is the same as saying that each fission at the time $\tau$ generates a $D H B F$ as from time $\tau$ to $T+t$ which is required. Assuming that the fission rate is constant over the interval as shown by Fig. 15.6, the following change of variable leads to the direct integration of the DHBF:

Decay heatevaluated by DHBF: $D H_{F}(t)=N_{F} \sigma_{f}^{F} \Phi \int_{t}^{T+t} D H B F_{F}\left(\tau^{\prime}\right) d \tau^{\prime}$

The total decay heat is obtained by summing on the nuclides that fission:

$$
D H(t)=\sum_{F} D H_{F}(t)
$$

For a load diagram modeled by steps $j$ for constant fission rates, the formula is extended by summing over the steps:

$$
D H(t)=\sum_{F} \sum_{j}\left(\begin{array}{lll}
N_{F} & \sigma_{f}^{F} & \Phi)_{j} \int_{\theta_{j+1}}^{\theta_{j}} D H B F_{F}(t-\theta) \quad d \theta \quad \text { with } \theta_{j+1}<\theta_{j}<0
\end{array}\right.
$$

It should be noted that the values of $\theta_{j}$ are negative in the above expression, in accordance with Fig. 15.7. The advantage of this method is that the only data required is the fission rates of heavy isotopes for each irradiation step of the core.

The $D H B F$ can be measured experimentally (Dickens ${ }^{5}$ in 1980, Akiyama ${ }^{6}$ in 1982, Fig. 15.8) using a very short irradiation period for a sample and expulsion in a

[^322]

Fig. 15.6 Decay heat burst function


Fig. 15.7 Decay heat for step load functions
calorimeter. However, the disadvantage of the method is that it does not account for the decay heat due to fission products during irradiation since the $D H B F$ are calculated in the absence of neutron flux. Correction for flux must be applied in order to improve the results.

### 15.6.4.3 Elementary Value Curves

The final method is an approach that differs slightly from $D H B F$, and is called the elementary value curves $(E V C)$ method. ${ }^{7}$ The principle is to calculate the fuel

[^323]

Fig. 15.8 Comparison of DHBF (with respect to cooling time) computed by DARWIN reference code with measures of Akiyama and Dickens (Courtesy CEA)
composition before irradiation of the reactor using a reduced depletion chain, which is assumed to be satisfactory with respect to precision on fuel composition, and then to calculate the decay heat response for each isotope in the fuel:

$$
D H(t)=\sum_{i \in f u e l} E V C_{i}(t)
$$

The elementary value curve for a quantity for fuel cycle $G$ (whether decay heat or any relevant physical quantity for the fuel cycle) for an isotope $i$ is the function giving the values of $G$ for $10^{20}$ atoms (an arbitrary reference value) for the isotope that decays naturally. The value of the $E V C$ for an isotope $i$ at time t is the value of the quantity $G$ of isotope $i$ and all its daughters that are present at time t :

$$
E V C_{i}^{G}(t)=G_{i}(t)+\sum_{i \rightarrow \ldots \rightarrow j} G_{j}(t)
$$

It should be noted that the $E V C$ of an isotope $i$ can be non-zero at a time $t$ even if its concentration is zero (albeit after complete disappearance of isotope $i$ ). Indeed, the $E V C$ takes into account the contributions of the daughters $j$ of the isotope $i$.

Similarly, the EVC may be increasing with time, as for ${ }^{137} C s$ with its daughter nucleus ${ }^{137 m} B a$, which has with a very short half-life and is in equilibrium with the
father isotope, resulting in a doubling effect of the activity (proportionally to the branching ratio), as described in Chap. 1. This effect is non-intuitive since decay heat is a decreasing function. This phenomenon of an increasing $E V C$ also exists for ${ }^{241} \mathrm{Pu}$ (Fig. 15.9).

This method has the advantage of accounting for the capture of fission products during irradiation via the fuel composition and thus the calculation of the fuel composition for isotopes with short periods and yet with significant contribution to decay heat, is not required. However, it is important to perform an analysis of the important isotopes for decay heat beforehand in a pre-calculation of EVC using a reference code (DARWIN from CEA in France). The gain in calculation time using this simplified method (lower than a second for the fuel) is very competitive compared to the reference codes, although it seems certain that future machines will render such methods obsolete.

### 15.6.4.4 Continuous Fission Curve Method

### 15.6.4.4.1 Principle

"On-line" computation of decay heat, i.e. during operation of the reactor, poses a difficult theoretical problem. Indeed, the fission energy is usually taken as 200 MeV


Fig. 15.9 EVC for the main heavy isotopes
per fission, and accounts for the stationary state of the energy due to $\gamma$ and $\beta$ decays of fission products. The decay heat is hence already taken into account in the fission energy if power is calculated as:

$$
P(t)=\kappa \Sigma_{f} \Phi(t)
$$

Moreover, a further 8 MeV is added to allow for the energy induced by the capture of other fission neutrons that do not contribute to the chain reaction. Consequently, all the energy released is counted in an elementary fission, even that which is released by radioactive decay or neutron capture. There is a problem if the neutron flux decreases with a kinetic process. In a theoretical case in which the flux tends towards 0 , the power decreases to 0 according to the previous formula. Yet, in a real case, there is still power due to the decay heat, which decreases slowly during cooling. This power heats up the coolant and this process is not usually taken into account in core calculation codes, even those dealing with reactor kinetics.

A simple method of addressing this problem is to consider the result of continuous fission in the reactor between time $\theta$ and current time $\tau$. For this time step, it is assumed that there is one fission per second continuously and that this fission immediately generates all the possible fission products according to their fission yields (which depend on the fissile nuclide considered). Infinite continuous fission is thus defined by taking the limit of the value of $\theta$ to $-\infty$. It is then assumed that the reactor stops instantaneously at time $\tau$, and the decay heat is calculated as a function of time $t$ after the reactor shuts down (Fig. 15.10).

The time origin is taken as the point at which the reactor shuts down, and the energy after continuous irradiation for a single fission before shut-down is given by the following (by noting that the values of $\theta$ during irradiation are negative):


Fig. 15.10 Infinite continuous fission

$$
Q_{1 \text { fission }}(t)=\int_{\theta=-\infty}^{\theta=0} D H B F(t-\theta) d \theta \equiv \operatorname{IDHBF}(t)
$$

This expression introduces the function IDHBF (for integrated DHBF), also called the Continuous Fission Curve (CFC). It may be noted that since the values of DHBF are in watts, the IDHBF, which are their integral over time, are given in joules (Fig. 15.11).

The decay heating due to a constant fission rate $\Sigma_{f} \Phi$ (in number of fissions per second) is obtained by multiplying it by the energy $Q_{1 \text { fission }}(t)$. The contribution of each fissile isotope $i$ is evaluated by summing for all fissile isotopes:

$$
D H(t)=\sum_{i \in\{f i s s i l e s\}} \Sigma_{f, i} \Phi \int_{\theta=-\infty}^{\theta=0} D H B F_{i}(t-\theta) d \theta=\sum_{i \in\{f i s s i l e s\}} \Sigma_{f, i} \Phi \operatorname{IDHBF} F_{i}(t)
$$

The variation per fission rate step is determined using a calculation shortcut. The contribution of a new power step, $\Sigma_{f}^{j} \Phi_{j}$ (the notations for summation are dropped for the sake of simplification), is computed by difference of the infinite fission curves between the beginning and the end of the step $\left[\theta_{j}, \theta_{j-1}\right]$ (Fig. 15.12):

$$
\begin{aligned}
\text { contribution }_{j}(t) & =\Sigma_{f}^{j} \Phi_{j}\left(\int_{\theta=-\infty}^{\theta=\theta_{j-1}} \operatorname{DHBF}(t-\theta) d \theta-\int_{\theta=-\infty}^{\theta=\theta_{j}} D H B F(t-\theta) d \theta\right) \\
& =\Sigma_{f}^{j} \Phi_{j}\left(\operatorname{IDHBF}\left(t-\theta_{j-1}\right)-\operatorname{IDHBF}\left(t-\theta_{j}\right)\right)
\end{aligned}
$$

The subtracted term corresponds to the contribution of the step prolonged at $-\infty$, which is implicitly accounted for in the continuous fission term IDHBF $\left(t-\theta_{j-1}\right)$. Since the times $\theta_{j}$ are negative, $t-\theta_{j-1}<t-\theta_{j}$, hence IDHBF $\left(t-\theta_{j-1}\right)>\operatorname{IDHBF}\left(t-\theta_{j}\right)$ and the contribution of the step is indeed positive. The successive steps $j$ before the reactor shuts down may be summed as follows:

Fig. 15.11 $\operatorname{IDHBF}(t)$ for $a$ fission by thermal neutron of U235 or Pu239



Fig. 15.12 Contribution of a step to decay heating

$$
D H(t)=\sum_{j=1}^{j=+\infty} \Sigma_{f}^{j} \Phi_{j}\left(I D H B F\left(t-\theta_{j-1}\right)-\operatorname{IDHBF}\left(t-\theta_{j}\right)\right)
$$

The further in the past each step is, the less significant its contribution.
This method is used in the COCCINELLE code for online calculation of the decay heat in the TREFLE simulator of the French EPR (Flamanville 3)

### 15.6.4.4.2 Capture Correction

While the major advantage of the infinite fission curve method is that it does not require isotopic depletion calculation, its main drawback is that it does not allow for the capture of fission products during irradiation. This capture effect depends on the flux level in the reactor and on the values of the capture cross-sections of the fission products. This effect can be pre-computed using a depletion code such as the CEA code DARWIN and a capture correction can be deduced and applied to the decay heat term of fission products during cooling. Studies have shown that capture correction depends more on the fluence (and thus burn-up) than on the flux level itself. Consequently, if the decay heating of fission products is computed at different burn-ups, the capture correction with time can be assumed as being independent of the flux level.

### 15.6.4.5 Calculation of Decay Sources and Their Spectrum

The number of decay particles- $\alpha, \beta$ or $\gamma-$ emitted by the $i$ th ray of an element of concentration $N(t)$ is proportional to activity as follows:

$$
G_{i}^{\alpha, \beta, \gamma}=\lambda_{\alpha, \beta, \gamma} N(t) \frac{I_{i}^{\alpha, \beta, \gamma}}{100}
$$

where $I_{i}^{\alpha, \beta, \gamma}$ is the intensity of the $i$ th ray in \%, obtained from nuclear data libraries such as JEF2. The total source is obtained by summing for all elements and the emission rays. Summing for a given energy mesh leads to a spectrum in \% of the total source.

The independent neutron source (not induced by a neutron flux) is calculated by accounting for the spontaneous fission $(F S)$ radioactive decay and $(\alpha, n)$ reactions for oxygen:

$$
S=S_{F S}+S_{(\alpha, n)}=\lambda_{F S} N(t) \sum_{i} \nu_{i}+\lambda_{\alpha} N(t) \sum_{i} r_{i}
$$

where $\nu_{\mathrm{i}}$ is the number of neutrons emitted by spontaneous fission in energy group $i$ and $r_{i}$ is the number of neutrons (yield) emitted by the reaction ( $\alpha, n$ ) in energy group $i$.

As $\alpha$ particles are roughly emitted with a 5 MeV energy by the fuel heavy nuclei, and because most of the $\alpha$ particles interact with the oxygen of the oxide fuel, a mean value of $3.3 \times 10^{-8}$ neutron per $\alpha$-Becquerel can be estimated, either for UOX or MOX fuels within a $10 \%$ margin.

The notion of spectrum is identical to that given for the $\alpha, \beta$ and $\gamma$ decays. R. Babut ${ }^{8}$ estimated the uncertainty on the inherent $(\alpha, n)$ sources computed by the integrated yield method as being more than $30 \%$.

### 15.6.5 Photon $\gamma$ and Neutron Dose Calculation

(Gambini and Granier 1986; Hine and Brownell, 1956, p. 10; Lilley, 2001, p. 181; Mayo 1998, p. 305; Shultis and Faw 2000, p. 121; Rockwell 1956, p. 17)

The absorbed dose is defined as the ratio of the mean energy deposited by ionizing particles in a given volume to the mass of the considered volume. The official unit of dose is the gray (symbol Gy) and corresponds to $1 \mathrm{~J} / \mathrm{kg}$. The specialists tend to use the older unit rad out of habit, or the CGS unit erg/g, for which the conversions are (Baur 1985, p. 48):

$$
1 \mathrm{gray}=100 \mathrm{rad}=10000 \mathrm{erg} / \mathrm{g}
$$

[^324]The dose calculation is carried out from the sources and spectra, as well as radiation protection data. For the $\gamma$ dose:

- the attenuation factor in the medium as a function of the energy of the $\gamma$ particle and the medium properties;
- the build-up factor that takes into account the contribution of scattered radiation and the distances travelled.

For neutron doses:

- scattering, capture, and total cross-sections of interaction with matter;
- accumulation factors.

Particles that are not directly ionizing, such as neutrons and photons, deposit their energy in matter in several ways:

- neutrons lose kinetic energy by colliding with atoms of matter (elastic or inelastic scattering),
- these particles create charged particles, for example by pair creation in the case of photons,
- the charged particles deposit their energy at sites other than the point of origin.

Hence, the notion of Kerma (Kinetic Energy Released in Matter) is employed in the field of radiation protection. Baur (1985, p. 49), Shultis and Faw (2000, p. 124) present the case of radiative capture in which the Kerma (which forms part of the field jargon) is equal to the recoil energy of the atom, which is the only charged particle formed. The deposited energy is the difference between the incident neutron energy, which by capture releases the binding energy for one nucleon in the compound nucleus, and the emitted photon energy, along with the recoil energy which is obtained completely as heat at the collision point:

$$
E_{\text {deposit }}=E_{\text {neutron }}+E_{\text {binding }}-h \nu-E_{\text {recoil }}=\text { Kerma }
$$

In this case, the Kerma and absorbed dose are similar. However, with Compton scattering, both the Compton electron and the scattered photon leave the considered volume, and the local dose is zero in the absence of Bremsstrahlung while the Kerma is equal to the kinetic energy of the Compton electron. Hence, the Kerma is larger than the absorbed dose in the latter case. In radiation protection codes, the Kerma is set as a cross section that depends on the material and incident particle energy, for which the reaction rate is the Kerma energy. Finally, the equivalent dose is a quantity that takes into account the damage caused by a particle, and allows comparison of the effects due to particles of different masses and energies. The equivalent dose is the product of the dose by a weighting (quality) factor $Q$ which ranges from 1 ( $X$-rays) to 20 (heavy recoiling atoms). It depends on the linear energy transfer of the particle and a second weighting factor $N$ that allows for the non-uniform distribution of the dose in space and energy, and is generally taken as 1 for internal sources that are ingested or inhaled (Baur 1985, p. 52).

$$
\text { Equivalent Dose }=\text { Dose. } Q . N
$$

The official unit of the equivalent dose is the sievert (symbol Sv), but for a dose expressed in rad, specialists use the rem, such that:

$$
1 \text { sievert }=100 \mathrm{rems}
$$

Dividing the dose (equivalent dose, resp.) by the exposure time gives the dose rate (equivalent dose rate, resp.). For example, the natural radiation due to natural radioactivity from Earth and cosmic rays is roughly equal to $100 \mathrm{mrem} / \mathrm{year}$ and industrial activities must not cause irradiation of more than $0.5 \mathrm{rem} / \mathrm{ye}$ ar for the public, while the authorized limit for nuclear personnel is $5 \mathrm{rem} / \mathrm{year}$. Weak doses continue to be the subject of heated debates, and these covered under the more general framework of the effects on the body of electromagnetic radiation (e.g. from mobile phones, etc.) (Bertin 1991).

It is common practice to represent the radiotoxicity for 1 kg of matter and by decay chain of heavy nuclides ( $4 \mathrm{n}, 4 \mathrm{n}+1,4 \mathrm{n}+2,4 \mathrm{n}+3$ ). The following figures set out the results of calculations performed by R. Gillet using the CEA MECCYCO code (1996, courtesy CEA) (Figs. 15.13, 15.14, 15.15, 15.16 and 15.17).

### 15.7 Isotopic Depletion Calculation

The Bateman equations can be solved analytically for simple cases, with examples being given in the following sections.


Fig. 15.13 Radiotoxicity for 1 kg of heavy isotopes of the 4 n chain (ICRP68 dose coefficients)


Fig. 15.14 Radiotoxicity for 1 kg of heavy isotopes of the $4 \mathrm{n}+1$ chain (ICRP68 dose coefficients)


Fig. 15.15 Radiotoxicity for 1 kg of heavy isotopes of the $4 \mathrm{n}+2$ chain (ICRP68 dose coefficients)

### 15.7.1 Chain-Decay Process: Recurrence Relations

(Bessis 1978, p. 46)
An analytical solution may be found in the case of a radioactive decay series (without isotopic coupling via the flux). Let us consider a decay chain of isotopes $N_{i}$ with radioactive decay constant $\lambda_{j}$ and with $n$ isotopes such that $N_{1} \rightarrow N_{2} \rightarrow \ldots \rightarrow N_{j} \rightarrow N_{j+1} \rightarrow \ldots \rightarrow N_{n}$. It may be assumed that the last isotope, $N_{n}$, is stable. The decay equations are as follows:


Fig. 15.16 Radiotoxicity for 1 kg of heavy isotopes of the $4 \mathrm{n}+3$ chain (ICRP68 dose coefficients)


Fig. 15.17 Decay/capture scheme for ${ }_{94}^{239} P u$

$$
\left\{\begin{array}{c}
\frac{d N_{1}}{d t}=-\lambda_{1} N_{1} \\
\frac{d N_{j+1}}{d t}=\lambda_{j} N_{j}-\lambda_{j+1} N_{j+1} \quad \text { for } i=1, n-1 \\
\frac{d N_{n}}{d t}=+\lambda_{n} N_{n}
\end{array}\right.
$$

Assuming that only the concentration of isotope $N_{1}$ is non-zero at time 0 and is equal to $N_{1}^{0}$, it can be shown that the calculation of the concentrations as a function of time, valid as of $j=2$, is:

$$
N_{j}=\sum_{i=1}^{j}\left(\frac{\prod_{k=1}^{j-1} \lambda_{k}}{\prod_{k=1, k \neq i}^{j}\left(\lambda_{k}-\lambda_{i}\right)} N_{1}^{0} e^{-\lambda_{i} t}\right)
$$

The proof is given by recurrence:
For $\quad j=1: \quad N_{1}=N_{1}^{0} e^{-\lambda_{1} t}$
For $\quad j=2: \quad \frac{d N_{2}}{d t}=\lambda_{1} N_{1}-\lambda_{2} N_{2}$
Thus: $\quad N_{2}=\frac{\lambda_{1}}{\lambda_{2}-\lambda_{1}} N_{1}^{0} e^{-\lambda_{1} t}+\frac{\lambda_{1}}{\lambda_{1}-\lambda_{2}} N_{1}^{0} e^{-\lambda_{2} t}$
which satisfies the recurrence for the first term. Since $\frac{d N_{j+1}}{d t}=\lambda_{j} N_{j}-\lambda_{j+1} N_{j+1}$, the solution is expressed as:

$$
N_{j+1}=\sum_{i=1}^{j+1} A_{i} e^{-\lambda_{i} t}
$$

Therefore:

$$
\begin{gathered}
\frac{d N_{j+1}}{d t}=\frac{d\left(\sum_{i=1}^{j+1} A_{i} e^{-\lambda_{i} t}\right)}{d t}=\sum_{i=1}^{j+1}\left(-\lambda_{i} A_{i} e^{-\lambda_{i} t}\right)=\lambda_{j} N_{j}-\lambda_{j+1} N_{j+1} \\
=\lambda_{j} \sum_{i=1}^{j}\left(\frac{\prod_{k=1}^{j-1} \lambda_{k}}{\prod_{k=1, k \neq i}^{j}\left(\lambda_{k}-\lambda_{i}\right)} N_{1}^{0} e^{-\lambda_{i} t}\right)-\lambda_{j+1}\left(\sum_{i=1}^{j+1} A_{i} e^{-\lambda_{i} t}\right) \\
\text { Hence: } \quad N_{j+1}=\sum_{i=1}^{j+1}\left(\frac{\prod_{k=1}^{j} \lambda_{k}}{\prod_{k=1, k \neq i}^{j+1}\left(\lambda_{k}-\lambda_{i}\right)} N_{1}^{0} e^{-\lambda_{i} t}\right)
\end{gathered}
$$

This formula assumes that all the values of $\lambda_{j}$ are different, implying the following:

- two different isotopes must not have strictly the same constants (fortunately, this is seldom the case, except for a very few isotopes);
- the decay chain must not loop over itself since the same isotope would be in the chain twice with different indices, which would lead to the previous case (similar constants).

$$
A_{1} \rightarrow \ldots \rightarrow A_{n} \rightarrow A_{1} \rightarrow A_{n+1} \rightarrow \ldots \text { is not allowed }
$$

This approach can be extended for cases with a neutron flux by grouping capture terms $\sigma \Phi$ with the decay constants, $\lambda$. However, in a true decay chain, which is arranged such that the $k t h$ isotope involves only the $k-1$ previous isotopes, the problem of looping is still possible due to $\alpha$ decay reactions. Indeed, by production of a ${ }_{2}^{4} \mathrm{He}$ atom, the isotope $A_{Z-2}^{A-4}$ is produced, and the chain loops over since this isotope also occurs earlier in the chain in order of increasing $Z$ and $A$. Fortunately, in the case of fission products, such decay reactions are negligible and can be ignored (in general, virtually no fission products emit $\alpha$ particles). For the decay chain of heavy nuclides, the $\alpha$ production of ${ }_{96}^{242} \mathrm{Cm}$ and ${ }_{96}^{244} \mathrm{Cm}$ can be taken into account by duplicating the daughter isotopes ${ }_{94}^{238} P u^{\text {bis }}$ and ${ }_{94}^{240} P u^{\text {bis }}$ to avoid looping. The calculation formula for the concentration $N_{j}$ of isotope $j$ can be extended by assuming that all values of $N_{j}^{0}$ are non-zero at time 0 . By noting that the Becquerel equations (i.e. the Bateman equations without flux) are linear, the same formula can be applied to the decay chain starting with $N_{2}$ to calculate the contribution from $N_{2}^{0}$ to $N_{j}$, denoted as $N_{j, 2}$ :

$$
N_{j, 2}=\sum_{i=2}^{j}\left(\frac{\prod_{k=2}^{j-1} \lambda_{k}}{\prod_{k=2, k \neq i}^{j}\left(\lambda_{k}-\lambda_{i}\right)} N_{2}^{0} e^{-\lambda_{i} t}\right)
$$

And so on for $N_{3}^{0}, \ldots N_{n-1}^{0}$. Finally:

$$
N_{j}=\sum_{p=1}^{p=j-1} N_{j, p}=\sum_{p=1}^{p=j-1} \sum_{i=2}^{j}\left(\frac{\prod_{k=p}^{j-1} \lambda_{k}}{\prod_{k=p, k \neq i}^{j}\left(\lambda_{k}-\lambda_{i}\right)} N_{p}^{0} e^{-\lambda_{i} t}\right)
$$

### 15.7.2 Case of Heavy Nuclides

The vector form of the Bateman equation for heavy nuclides is expressed as:

$$
\frac{d \vec{N}(t)}{d t}=A \vec{N}(t)
$$

where $A$ is a matrix of dimension $\operatorname{order}(A)$.
Several numerical methods can be used to solve this linear differential equation. In general, the Runge-Kutta method of order 4 is often utilized. However, since
$A$ depends on time during depletion under flux, we may use the finite difference method, which, though more onerous in terms of computational time, is very simple to implement. There is also the matrix exponential method (Varga 1962), which highlights the matrix properties of the Bateman system. The solution to this vector differential equation is expressed as:
$\vec{N}(t)=e^{A t} \vec{N}(o)$ where $e^{A t}$ is the exponential of the matrix $A t$.
Using a Taylor expansion, the matrix exponential is defined as:

$$
e^{A t} \approx\left(I+A t+\frac{(A t)^{2}}{2!}+\ldots+\frac{(A t)^{n}}{n!}\right)
$$

Thus, $e^{A t}$ can be computed by choosing an intermediate variable $\theta=t / 2^{m}$, such that the spectral radius of the matrix $A \theta$ is negligible compared to 1 , i.e. $\|A \theta\| \leq 1$ so that the Taylor expansion of $e^{A \theta}$ at a finite order is warranted. $e^{A t}$ is obtained by taking the result of $e^{A \theta}$ to the power of $2^{m}$. The spectral radius of the matrix is usually difficult to compute directly, but it can be bounded by a maximum quite easily. Squaring the matrix successively consists in evaluating the products $\sum a_{i j} a_{j k}$, which is also denoted as $a_{i j} a_{j k}$ in Einstein notation. The convergence of this squaring process is ensured if every element of the product is always smaller than 1 at each step, i.e.:

$$
\max (|A|)=\max _{i}\left(\max _{j}\left(\left|a_{i j}\right|\right)\right)
$$

Thus, it can be guaranteed that:

$$
\|\mathrm{A}\| \leq \max _{i, k}\left(a_{i j} \cdot a_{j k}\right) \leq \max _{i, k}\left(\left|a_{i j}\right| \cdot\left|a_{j k}\right|\right) \leq \operatorname{order}(A) \cdot(\max (|A|))^{2}
$$

Therefore, we obtain a (highly conservative!) upper bounding value for the spectral radius of $A$, and hence also for that of $A \theta$.

$$
\left.\frac{t}{2^{m}} \times \max _{i, k}\left|a_{i j} \| a_{j k}\right| \leq \frac{t}{2^{m}} \operatorname{order}(A) \max (|A|)\right)^{2} \leq 1
$$

The situation of activation products is similar to that of heavy nuclides due to their identical form in the Bateman equation system.

### 15.7.3 Case of Fission Products

The vector form for the Bateman equation for fission products is written as:

$$
\frac{d \vec{N}(t)}{d t}=A \vec{N}(t)+S
$$

with the solution expressed as:

$$
\vec{N}(t)=\underbrace{e^{A t}}_{B(t)} \vec{N}(o)+\underbrace{\left(e^{A t}-I\right) A^{-1}}_{c(t)} S
$$

Thus: $\left\{\begin{array}{c}\frac{d \vec{N}}{d t}=A e^{A t} \vec{N}(o)+A e^{A t} A^{-1} S \\ A \vec{N}(t)+S=A e^{A t} \vec{N}(o)+A e^{A t} A^{-1} S-\underbrace{A I A^{-1}}_{I} S+S=\frac{d \vec{N}}{d t}\end{array}\right.$
It can be seen that: $B(t)=C(t) A+I$. Since:

$$
\begin{aligned}
C(2 t) & =\left(e^{A 2 t}-I\right) A^{-1}=\left(e^{A t}-I\right)\left(e^{A t}+I\right) A^{-1}=\left(e^{A t}+I\right) C(t) \\
& =(B(t)+I) C(t) .
\end{aligned}
$$

By setting $\theta=t / 2^{m}, B(\theta)$ can be evaluated using a Taylor expansion of $C(\theta)$ obtained through an initial expansion of $B(\theta)$ :

$$
\left\{\begin{array}{c}
B(\theta)=I+A \theta+\frac{(A \theta)^{2}}{2!}+\ldots+\frac{(A \theta)^{n}}{n!} \\
C(\theta)=(B(\theta)-I)) A^{-1}=\theta\left[I+\frac{A \theta}{2!}+\ldots+\frac{(A \theta)^{n-1}}{n!}\right]
\end{array}\right.
$$

$B$ and $C$ can then be determined sequentially to obtain the values of $B\left(2^{m} \theta\right)=B(t)$ and $C\left(2^{m} \theta\right)=C(t)$. Thus:

$$
\vec{N}(t)=\vec{N}\left(2^{m} \theta\right)=B\left(2^{m} \theta\right) \cdot \vec{N}(0)+C\left(2^{m} \theta\right) \cdot S
$$

### 15.7.4 Reference Composition of Some PWR Fuel

Below are the mass compositions of two reference fuels. The first is a uranium oxide fuel enriched at $3.7 \%$ (quarter core fuel management), and the second a mixed oxide MOX fuel with a plutonium content of $5.3 \%$ (equivalent to a UOX $3.25 \%$ with a one-third core fuel management). The mass of metal is given for an assembly. It can be seen that second-generation plutonium (obtained from eventual MOX recycling) is fairly degraded (less fissile isotopes compared to the amount of absorbing isotopes such as plutonium 242). The use of second-generation plutonium is thus not possible

Table 15.3 UOX 3.7\% fuel: uranium and plutonium content

| Uranium enriched at 3.7\% ( $1 / 4$ core fuel management) |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $\begin{aligned} & \text { Loaded } \\ & (\%) \end{aligned}$ | $\begin{array}{\|l\|} \hline \text { Burn-up } \\ 42,000 \mathrm{MWd} / \mathrm{t} \end{array}$ (\%) | 42,000 MWd/t, cooled for 3 years (\%) | $42,000 \mathrm{MWd} / \mathrm{t}$, cooled for 3 years, recycled, cooled for a further 2 years (\%) |
| ${ }_{92}^{234} \mathrm{U}$ | 0.034 | 0.020 | 0.020 | 0.020 |
| ${ }_{92}^{235} \mathrm{U}$ | 3.7 | 0.864 | 0.864 | 0.864 |
| ${ }_{92}^{236} \mathrm{U}$ | 0 | 0.505 | 0.505 | 0.505 |
| ${ }_{92}^{238} \mathrm{U}$ | 96.266 | 98.612 | 98.612 | 98.612 |
| U Total | 100 | 100 | 100 | 100 |
| ${ }_{94}^{238} \mathrm{Pu}$ | 0 | 2.621 | 2.722 | 2.745 |
| ${ }_{94}^{239} \mathrm{Pu}$ | 0 | 53.266 | 53.187 | 54.498 |
| ${ }_{94}^{240} \mathrm{Pu}$ | 0 | 22.277 | 22.288 | 22.837 |
| ${ }_{94}^{241} \mathrm{Pu}$ | 0 | 14.566 | 12.588 | 11.715 |
| ${ }_{95}^{241} \mathrm{Am}$ | 0 | 0.408 | 2.363 | 1.184 |
| ${ }_{94}^{242} \mathrm{Pu}$ | 0 | 6.862 | 6.852 | 7.021 |
| Pu total | - | 100 | 100 | 0 |

(in any case not with a depleted uranium support) due to the fact that the increasing plutonium content is near the safety limits (Tables 15.3, 15.4, 15.5 and 15.6).

### 15.8 Decay Chain Reduction Principle

In order to optimize computation times, not all available isotopes are used in industrial fuel cycle analysis. The decay/capture chains are reduced to take into account the most significant phenomena or the isotopes of interest, whence the notion of simplified chains. Chain reduction is a complex physical problem that requires detailed fuel cycle analysis, as it depends on the quantity that we are seeking to evaluate. For instance, an isotope with a very short period has a high activity at the beginning of life but at the same time, it disappears very quickly and does not contribute significantly to the mass balance. Consequently, it is recommended that every hypothesis used in chain reductions be set out in detail so as to avoid dangerous mistakes.
Table 15.4 UOX 3.7\% fuel: uranium and plutonium content

| Uranium enriched at 3.7\% (1/4 core fuel management): heavy nuclides content |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Loaded (\%) | Loaded $(\mathrm{Kg})$ | $\begin{aligned} & 42,000 \mathrm{MWd} / \\ & \mathrm{t}(\%) \end{aligned}$ | $\begin{aligned} & 42,000 \mathrm{MWd} / \\ & \mathrm{t}(\mathrm{~kg}) \end{aligned}$ | 42,000 MWd/ <br> t , cooled for <br> 3 years (\%) | 42,000 MWd/ <br> $t$, cooled for <br> 3 years (kg) | 42,000 MWd/t, cooled for 3 years, recycled, cooled for a further 2 years (\%) | 42,000 MWd/t, cooled for 3 years, recycled, cooled for a further 2 years ( kg ) |
| ${ }_{92}^{234} \mathrm{U}$ | 0.034 | 0.138 | 0.020 | 0.088 | 0.020 | 0.088 | 0.020 | 0.088 |
| ${ }_{92}^{235} \mathrm{U}$ | 3.7 | 14.986 | 0.852 | 3.762 | 0.853 | 3.762 | 0.854 | 3.762 |
| ${ }_{92}^{236} \mathrm{U}$ | 0 | 0 | 0.498 | 2.198 | 0.498 | 2.198 | 0.499 | 2.198 |
| ${ }_{92}^{238} \mathrm{U}$ | 96.266 | 446.132 | 97.338 | 429.568 | 97.339 | 429.568 | 96.461 | 429.568 |
| ${ }_{93}^{237} \mathrm{~Np}$ | 0 | 0 | 0.075 | 0.332 | 0.075 | 0.332 | recycled | 0 |
| ${ }_{94}^{238} \mathrm{Pu}$ | 0 | 0 | 0.031 | 0.138 | 0.033 | 0.143 | 0.032 | 0 |
| ${ }_{94}^{239} \mathrm{Pu}$ | 0 | 0 | 0.635 | 2.803 | 0.633 | 2.803 | 0.636 | 0 |
| ${ }_{94}^{240} \mathrm{Pu}$ | 0 | 0 | 0.266 | 1.172 | 0.266 | 1.175 | 0.267 | 0 |
| ${ }_{94}^{241} \mathrm{Pu}$ | 0 | 0 | 0.174 | 0.767 | 0.150 | 0.664 | 0.137 | 0 |
| ${ }_{95}^{241} \mathrm{Am}$ | 0 | 0 | 0.005 | 0.021 | 0.028 | 0.125 | 0.014 | 0 |
| ${ }_{94}^{242} \mathrm{Pu}$ | 0 | 0 | 0.082 | 0.361 | 0.082 | 0.361 | 0.002 | 0 |
| ${ }_{95}^{242 m} \mathrm{Am}$ | 0 | 0 | 0 | 0 | 0 | 0 | recycled | 0 |
| ${ }_{96}^{242} \mathrm{Cm}$ | 0 | 0 | 0.002 | 0.009 | 0 | 0 | recycled | 0 |
| ${ }_{95}^{243} \mathrm{Am}$ | 0 | 0 | 0.017 | 0.074 | 0.017 | 0.0743 | recycled | 0 |
| ${ }_{96}^{244} \mathrm{Cm}$ | 0 | 0 | 0.005 | 0.021 | 0.004 | 0.019 | recycled | 0 |
| $\begin{aligned} & \text { Pu } \\ & \text { total + Am241 } \end{aligned}$ | 0 | 0 | 1.192 | 5.262 | 1.194 | 5.270 | 1.167 | 5.143 |
| Pu total | 0 | 0 | 1.188 | 5.242 | 1.166 | 5.146 | 1.153 | 5.082 |
| U total | 100 | 461.256 | 98.709 | 435.616 | 98.709 | 435.616 | 98.833 | 435.616 |
| Others | 0 | 0 | 0.104 | 0.458 | 0.125 | 0.550 | 0.014 | 0.061 |
| TOTAL | 100 | 461.256 | 100 | 441.315 | 100 | 441.311 | 100 | 440.759 |

Table 15.5 MOX 5.3\% fuel: uranium and plutonium content
$M O X$ at $5.30 \%$ ( $1 / 3$ core fuel management)

|  | Loaded (\%) | $\begin{aligned} & 35,000 \mathrm{MWd} / \mathrm{t} \\ & (\%) \end{aligned}$ | 35,000 MWd/t, cooled 3 years (\%) | 35,000 MWd/t, cooled 3 years, recycled, cooled further 2 years (\%) |
| :---: | :---: | :---: | :---: | :---: |
| ${ }_{92}^{234} \mathrm{U}$ | 0 | 0 | 0 | 0 |
| ${ }_{92}^{235} \mathrm{U}$ | 0.225 | 0.117 | 0.117 | 0.117 |
| ${ }_{92}^{236} \mathrm{U}$ | 0 | 0.024 | 0.024 | 0.024 |
| $\begin{array}{r} 238 \\ \hline 92 \\ \hline \end{array}$ | 99.775 | 99.860 | 99.860 | 99.860 |
| $\begin{aligned} & \hline \mathbf{U} \\ & \text { Total } \end{aligned}$ | 100 | 100 | 100 | 100 |
| ${ }_{94}^{238} \mathrm{Pu}$ | 1.829 | 2.714 | 3.028 | 3.095 |
| ${ }_{94}^{239} \mathrm{Pu}$ | 57.933 | 40.695 | 40.506 | 42.057 |
| ${ }_{94}^{240} \mathrm{Pu}$ | 22.501 | 27.330 | 27.341 | 28.388 |
| ${ }_{94}^{241} \mathrm{Pu}$ | 11.061 | 17.87 | 15.601 | 14.525 |
| ${ }_{95}^{241} \mathrm{Am}$ | 1.080 | 1.255 | 3.641 | 1.468 |
| ${ }_{94}^{242} \mathrm{Pu}$ | 5.596 | 10.130 | 10.083 | 10.469 |
| Pu total | 100 | 100 | 100 | 0 |

### 15.8.1 Heavy Nuclide Chain for Reactivity Calculations of Reactors

In this case, the quantity of interest is mainly the reactivity of the fuel (its ability to produce energy). Thus the nuclear reactions of the main isotopes undergoing fission must be described with sufficient precision to enable satisfactory estimation of the mass balance of heavy absorbing nuclides. Figure 15.18 shows a decay/capture chain corresponding to the recommended library SERMA79 which was historically used by $C E A$ and $E D F$ until the end of the 1990s. A recommended library is a qualified set of nuclear data associated with a simplified chain. The SERMA79 decay chain was developed to provide a reactivity balance as close as possible to the full chain; the isotopes in the library accounted for $99 \%$ of total absorption. However, the mass balance is not very precise since many isotopes are missing from the library. The products of the $\alpha$ decays of the curium isotopes were fixed to "duplicated" plutonium isotopes to avoid looping of chains, which was not supported by the APOLLO1 code. This historical chain contained 15 heavy isotopes, starting from ${ }_{92}^{234} \mathrm{U}$ and ending with ${ }_{96}^{244} \mathrm{Cm}$. It did not contain any thorium isotope or ${ }_{92}^{233} U$, and a separate chain is thus required for reactors with this particular fuel.
Table 15.6 MOX 5.3\% fuel: uranium and plutonium content

|  | Loaded (\%) | Loaded $(\mathrm{Kg})$ | $\begin{aligned} & 35,000 \mathrm{MWd} / \mathrm{t} \\ & (\%) \end{aligned}$ | $\begin{aligned} & 35,000 \mathrm{MWd} / \mathrm{t} \\ & (\mathrm{~kg}) \end{aligned}$ | 35,000 MWd/t, cooled for 3 years (\%) | 35,000 MWd/t on, cooled for 3 years (kg) | 35,000 MWd/t, cooled for 3 years, recycled, cooled for a further 2 years (\%) | 35,000 MWd/t, cooled for 3 years, recycled, cooled for a further 2 years (kg) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ${ }_{92}^{234} \mathrm{U}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| ${ }_{92}^{235} \mathrm{U}$ | 0.213 | 0.983 | 0.111 | 0.496 | 0.111 | 0.496 | 0.112 | 0.496 |
| ${ }_{92}^{236} \mathrm{U}$ | 0 | 0 | 0.023 | 0.101 | 0.023 | 0.101 | 0.023 | 0.101 |
| ${ }_{92}^{238} \mathrm{U}$ | 94.487 | 435.870 | 95.406 | 424.392 | 95.409 | 424.392 | 95.763 | 424.392 |
| ${ }_{93}^{237} \mathrm{~Np}$ | 0 | 0 | 0.022 | 0.098 | 0.022 | 0.098 | recycled | 0 |
| ${ }_{94}^{238} \mathrm{Pu}$ | 1.83\% | 0.447 | 0.115 | 0.510 | 0.129 | 0.572 | 0.127 | 0.563 |
| ${ }_{94}^{239} \mathrm{Pu}$ | 57.8\% | 14.136 | 1.719 | 7.647 | 1.719 | 7.647 | 1.725 | 7.647 |
| ${ }_{94}^{240} \mathrm{Pu}$ | 22.5\% | 5.501 | 1.154 | 5.135 | 1.160 | 5.162 | 1.165 | 25.16 |
| ${ }_{94}^{241} \mathrm{Pu}$ | 11.06\% | 2.704 | 0.755 | 3.359 | 0.654 | 2.907 | 0.596 | 2.641 |
| ${ }_{95}^{241} \mathrm{Am}$ | 1.08\% | 0.264 | 0.053 | 0.236 | 0.155 | 0.687 | 0.060 | 0.267 |
| ${ }_{94}^{242} \mathrm{Pu}$ | 5.60\% | 1.368 | 0.428 | 1.904 | 0.428 | 1.904 | 0.430 | 1.904 |
| ${ }_{95}^{242 m} \mathrm{Am}$ | 0 | 0 | 0.001 | 0.005 | 0.001 | 0.005 | recycled | 0 |
| ${ }_{96}^{242} \mathrm{Cm}$ | 0 | 0 | 0.017 | 0.077 | 0.0002 | 0.001 | recycled | 0 |
| ${ }_{95}^{243} \mathrm{Am}$ | 0 | 0 | 0.140 | 0.623 | 0.140 | 0.623 | recycled | 0 |
| ${ }_{96}^{244} \mathrm{Cm}$ | 0 | 0 | 0.055 | 0.245 | 0.049 | 0.219 | recycled | 0 |
| $\begin{aligned} & \text { Pu } \\ & \text { total + Am241 } \end{aligned}$ | 5.30 | 24.448 | 4.224 | 18.790 | 4.244 | 18.878 | 4.103 | 18.182 |
| Pu total | 5.242 | 24.184 | 4.171 | 18.555 | 4.090 | 18.191 | 4.042 | 17.915 |
| U total | 94.700 | 436.852 | 95.540 | 424.988 | 95.543 | 424.988 | 95.897 | 424.988 |
| Others | 0.057 | 0.264 | 0.289 | 1.284 | 0.367 | 1.633 | 0.060 | 0.267 |
| TOTAL | 100 | 461.300 | 100 | 444.827 | 100 | 444.812 | 100 | 443.170 |



Fig. 15.18 Decay chain for heavy nuclides from the SERMA79 recommendation

### 15.8.1.1 Numerical Example: Plutonium Production in a Uranium Fuel Assembly

Let us consider a 900 MWe reactor with a specific power of $38.3 \mathrm{MW} / \mathrm{t}$ containing 157 fuel assemblies with 461.4 kg (metal) of uranium oxide enriched at $3.25 \%$. The aim is to determine the amount of ${ }_{94}^{239} \mathrm{Pu}$ produced after a relatively short time period, e.g. $10 E F P D$. The production scheme for ${ }_{94}^{239} P u$ is as follows:

The associated Bateman equation for this chain is given by:

$$
\begin{aligned}
& \left.\left.-\sigma \underset{94}{(n, 2 n)} \underset{94}{(n,}{ }_{94}^{239} P u\right] . \Phi+\sigma \underset{94}{(n, \gamma)} \underset{94}{(2388} P u\right] . \Phi
\end{aligned}
$$

Using the data from Tables 15.7 and 15.8 and considering that $\sigma_{(n, 2 n)}{ }^{2399} P u=0.001$ barn, the amount of ${ }_{94}^{239} \mathrm{Pu}$ produced by capture reactions of ${ }_{92}^{238} U$ can be evaluated under the following assumptions:

- $\lambda_{239} P u \quad\left[{ }_{94}^{239} P u\right]$ is negligible due to the very long period of ${ }_{94}^{239} P u$.

Table 15.7 Main cross sections for uranium and plutonium isotopes

|  | 235 <br> 92 | 238 <br> 92 | ${ }_{94}^{238} P u$ | ${ }_{94}^{239} P u$ |
| :--- | :--- | :--- | :--- | :--- |
| $\sigma_{f[\text { barn }]}$ | 45.11 | 0.101 | 2.48 | 116 |
| $\sigma_{a[\text { barn }]}$ | 54.84 | 0.984 | 35.29 | 183 |

Table 15.8 Main periods for uranium and plutonium isotopes

|  | ${ }_{92}^{238} \mathrm{U}$ | ${ }_{92}^{239} \mathrm{U}$ | ${ }_{93}^{239} \mathrm{~Np}$ | ${ }_{94}^{238} \mathrm{Pu}$ | ${ }_{94}^{239} \mathrm{Pu}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| T (half-life) | $4.468 \times 10^{9}$ years | 23 min | 2.3 days | 88 years | 24,110 years |

- $\left.\sigma_{94}^{(n, 2 n)} \underset{94}{(n, 239} P u{ }_{94}^{239} P u\right] \Phi$ is negligible since the $(n, 2 n)$ cross section of ${ }_{94}^{239} P u$ is very small. The same applies for $\sigma_{234}^{(n, \gamma)} \underset{94}{\left({ }_{94}\right)}\left[{ }_{94}^{238} P u\right] \Phi$.

Since ${ }_{92}^{239} \mathrm{U}$ and ${ }_{93}^{239} N p$ have very short periods, the production rate of ${ }_{94}^{239} \mathrm{Pu}$ can be considered the capture rate of ${ }_{92}^{238} U$ by chain simplification.

$$
\begin{aligned}
& \lambda_{239} N p\left[{ }_{93}^{239} N p\right]=\sigma \underset{92}{(n, \gamma)} \quad\left[\begin{array}{c}
238 \\
{ }_{93} U 8
\end{array}\left[\begin{array}{c}
{ }_{92} U
\end{array}\right] \Phi\right.
\end{aligned}
$$

As the fuel assembly contains a large amount of ${ }_{92}^{238} U(461.4 \times 0.0325=$ 14.9955 kg of ${ }_{92}^{235} U$ and $461.4 \times 0.9675=446.4045 \mathrm{~kg}$ of ${ }_{92}^{238} U$ ), it may be assumed that its concentration varies only slightly over 10 days. The flux is also assumed to be constant and can be evaluated by considering that it is caused only by thermal fission of ${ }_{92}^{235} U$ and fast fission of ${ }_{92}^{238} U$ :

$$
\Phi=\frac{\text { POWER relased by a tonne }}{\text { FISSION induced in the same tonne }}=\frac{P}{k \sum_{i \in f i s s i l e s} N_{i} \sigma_{f_{i}}}
$$

A mean fission energy value of 200 MeV /fission is chosen, which also includes the energy of approximately $\nu-1$ captured neutrons. The calculation is applied for 1 ton of heavy metal (on the basis of 461.4 kg per assembly, the power released is not 38.3 MW but rather $38.3 \times 0.4614=17.67 \mathrm{MW}$ ). Since the number of fissile atoms also includes the 0.4614 coefficient, it simplifies out.

$$
\begin{aligned}
& \Phi=\frac{38.310^{6} \mathrm{Watt}}{200 \mathrm{MeV} \times 10^{6} \frac{\mathrm{eV}}{\mathrm{MeV}} \times 1.610^{-19} \frac{\mathrm{Joule}}{e V}[N_{U 235} \times \underbrace{45.1110^{-24} \mathrm{~cm}^{2}}_{\sigma_{U 235}}+N_{U 238} \times \underbrace{0.10110^{-24} \mathrm{~cm}^{2}}_{\sigma_{f U 238}}]} \\
& \left\{\begin{array}{l}
N_{U 235}=\frac{32.5 \mathrm{~kg}}{23510^{-3} \mathrm{~kg} \cdot \mathrm{~mol}^{-1}} \times 6.02210^{23}=8.32968110^{25} \text { atoms of } U_{235} \text { per tonne } \\
N_{U 238}=\frac{967.5 \mathrm{~kg}}{23810^{-3} \mathrm{~kg} \cdot \mathrm{~mol}^{-1}} \times 6.02210^{23}=2.44842510^{27} \text { atoms of } U_{238} \text { per tonne }
\end{array}\right.
\end{aligned}
$$

Thus: $\Phi=2.98859410^{14}$ neutron. $\mathrm{cm}^{-2} \cdot \mathrm{~s}^{-1} \approx 3.010^{14}$ neutron. $\mathrm{cm}^{-2} \cdot \mathrm{~s}^{-1}$
It can be seen that the number of fissions of ${ }_{92}^{235} U$ is more than tenfold that of ${ }_{92}^{238} U$, although ${ }_{92}^{238} U$ has a much higher concentration:

$$
\frac{U_{238} \text { fission }}{U_{235} \text { fission }}=\frac{247.29 \text { fission }}{3757.52 \text { fission }} \approx 6.6 \%
$$

Most fission reactions occur from ${ }_{92}^{235} U$ although there is 30 times less ${ }_{92}^{235} U$ than ${ }_{92}^{238} U$. It should be pointed out that ${ }_{92}^{238} U$ is fissile only in the fast energy spectrum, thereby explaining its low cross section for one energy group. The simplified ${ }_{94}^{239} P u$ equation is written as:

The resulting equation is a first-order differential equation that can be integrated as the sum of a general solution to a homogeneous differential equation and a particular solution of the inhomogeneous equation. A trivial particular solution to the inhomogeneous equation is:

$$
\left[{ }_{94}^{239} P u\right]=\frac{\sigma_{238}^{(n, \gamma)}}{{ }_{92}^{a b s} U}\left[{ }_{92}^{238} P u\right]
$$

The general solution to the homogeneous equation is given by: $\left[{ }_{94}^{239} P u\right]=$ $A e-\sigma{ }_{94}^{a 39} P u$. $\Phi t$ with an initial value of: $\left[{ }_{94}^{239} P u\right](0)=0$. Thus, the solution to the differential equation is:

$$
\left[{ }_{94}^{239} P u\right](t)=\frac{\sigma_{29}^{(n, \gamma)}}{\underset{{ }_{92}}{a b s} U}\left[{ }_{94}{ }_{92}^{239} U u\right]_{0} \quad\left(1-e^{-\sigma_{234}^{a b s} P u} \quad \Phi t\right)
$$

Thus, the production of ${ }_{94}^{239} P u$ is 0.111 kg per fuel assembly after $10 E F P D$. If the calculation for ${ }_{94}^{239} \mathrm{Pu}$ is carried out for longer time periods, the isotopic change must be allowed as well as the production/use-up terms (Fig. 15.19).

### 15.8.1.2 Decay Chain for Heavy Nuclides and Fission Products from the SERMA79 Recommendation

This recommendation (Fig. 15.18), established by the CEA/SERMA at the end of the 1970s, includes a chain of 77 important fission products for neutron capture (Figs. 15.20, 15.21, and 15.22). The relevant choice of fission products allows for $95 \%$ of the total absorption as computed for 699 fission products. It can be noted that by taking twice the number of isotopes (chain with 154 fission products called incineration chain), $99.9 \%$ of the total absorption is obtained (Fig. 15.23).


Fig. 15.19 Capture of ${ }_{95}^{241} \mathrm{Am}$


Fig. 15.20 Decay chain with 77 fission products from zirconium to indium


Fig. 15.21 Decay chain with 77 fission products from cerium to gadolinium


Fig. 15.22 Decay chain with 77 fission products from tellurium to lanthanum


Fig. 15.23 REL2005 decay chain for heavy nuclides. Since all heavy nuclides being fissile, fission arrows are not shown

### 15.8.1.3 Decay Chain of Heavy Nuclides from the REL2005 Recommendation

This recommendation REL2005 (Fig. 15.23) was created at the beginning of the 2000s with nuclear data stemming from JEFF3 for use by the APOLLO2 code. It is used at $E D F$ for the new calculation chain ANDROMEDE.

The capture of ${ }_{95}^{241} \mathrm{Am}$ is complex since it produces $15 \%$ of ${ }_{95}^{242 \mathrm{~m}} \mathrm{Am}$ and $85 \%$ of ${ }_{95}^{242} \mathrm{Am} .{ }_{95}^{242 m} \mathrm{Am}$ is itself radioactive and emits $\gamma$ particles (by isomeric transition), decaying thus into ${ }_{95}^{242} \mathrm{Am}$.

Erreur! Référence non valide pour un signet.


Fig. 15.24 Chain reduction for fission products of same mass number (isobars)

### 15.8.2 Decay Chain Reduction

Chain reduction should always be carried out for a given fuel cycle application. Let us consider the heavy nuclides that disintegrate by $\alpha$ decay as follows:

The decay chain is reduced as shown by Fig. 15.24 by eliminating the intermediate $\alpha$ emitter, which has a very short period and would require a longer calculation time. This logic is applicable when only the mass balance is required (since the intermediate emitter will be present for a very short time period). However, it cannot be applied for activity: if the isotope disappears quickly, it has a very short period and thus a high decay constant $\lambda$. The activity being the product of $\lambda$ (high) and the concentration $N$ (low), it is possible that this emitter has a significant activity. The concentration of the isotope is no longer available by chain reduction and its activity cannot be evaluated. Using the same logic as the mass balance, a decay chain of fission products can be simplified using the cumulated yield of an isotope set at the head of the chain (Fig. 15.25).

However, in the case of decay with branching, reduction should be carried out carefully for the independent yields that are carried forward. The successive reduction of the ${ }_{34}^{79} \mathrm{Se}$ chain is very informative in this regard.

### 15.8.2. $\quad{ }_{34}^{79} \mathrm{Se}$ Chain Reduction

The complete model (from JEF2) for the decay/capture scheme of ${ }_{34}^{79} \mathrm{Se}$ is given Fig. 15.26:

A first reduction is carried out on the exact model using a "long-period" logic: ${ }_{34}^{79 m} \mathrm{Se}$ is eliminated (Fig. 15.27):

In the final reduction, ${ }_{35}^{80} \mathrm{Br}$ is eliminated (Fig. 15.28):


Fig. 15.25 Chain reduction for mass balance


(17.4 min)


Fig. 15.26 Reference chain of ${ }_{34}^{79} \mathrm{Se}$


Fig. 15.27 Reduced chain of ${ }_{34}^{79} \mathrm{Se}$ (1st step)


Fig. 15.28 Reduced chain of ${ }_{34}^{79} \mathrm{Se}$ (2nd step)

### 15.9 Activation: The Example of Control Rods

In industrial reactors such as water reactors, core reactivity is controlled using control rods manufactured from absorbing materials such as a mixture of silver-indium-cadmium ( $80 \%, 15 \%, 5 \%$ by mass) or boron carbide ( $B_{4} C$ ). These rods can be inserted in the core (during automatic shut-down or in some operating modes), and are thus irradiated by the neutron flux over several cycles (unlike fuel assemblies, which remain in the core for 3 to 4 cycles, control rods have a longer lifetime of up to $10-15$ cycles). The control rods are replaced in the event of mechanical problems (wear-out) or abnormal swelling at the end of the rod (which is subjected to a flux even when the rods are extracted since the lower end is just above the active core) caused by the formation of tin ( Sn ) due to the activation of indium. The activation chain of a silver-indium-cadmium rod is very complex but it can be reduced under physical considerations by using a "long-period" logic and by taking into account the product of the cross sections and the neutron flux (the cross section is taken at $2200 \mathrm{~m} / \mathrm{s}$ if no other one-group value is available for the considered spectrum) and comparing it to the decay constant, $\lambda$. For a given isotope, the cross section and flux product against $\lambda$ comparison is generally ruled out with respect to each other for a 100 -fold ratio. When the cross section is very small, the decay chains can be uncoupled, thereby making physical analysis simpler. In this case, it is seen that the main production of $\operatorname{tin}\left({ }_{50}^{116} \mathrm{Sn}\right)$ arises from the use-up of ${ }_{59}^{115} \mathrm{In}$ (Fig. 15.29).


Fig. 15.29 Simplified silver-indium-cadmium chain

Fig. 15.30 Xenon
135 production chain


### 15.10 Xenon Physics

### 15.10.1 Production of Xenon

Xenon is a noble gas with a radioactive isotope ${ }_{54}^{135} X e$ that is produced directly by fission and also mainly by $\beta^{-}$decay of the isotope ${ }_{53}^{135} \mathrm{I}$. The latter is also a fission product produced in much larger quantities (to be more precise, ${ }_{53}^{135} I$ is the decay product of ${ }_{52}^{135} \mathrm{Te}$, which decays by emitting $\beta^{-}$with a 1-min half-life, and is thus neglected in the chain using the cumulated yield of iodine).

The major drawback of ${ }_{54}^{135} \mathrm{Xe}$ is that it is highly absorbing under thermal flux. It has a very wide resonance:
$\left(\sigma^{(n, \gamma)}{ }_{2200 \mathrm{~m} / \mathrm{s}}=2653040 \text { barns, } I^{(n, \gamma)}=7664 \text { barns }\right)^{9}$ at low energy $(0.07 \mathrm{eV})$. Furthermore, it is still produced by the radioactivity of the father isotope, ${ }_{53}^{135} I$ (half-life of $6.61 \mathrm{~h}, \lambda_{I}=2.913 \quad 10^{-5} \mathrm{~s}^{-1}$ ) even after reactor shutdown, and has a large enough reactivity effect to choke the reactor (Fig. 15.30).

This production is compensated after some time by the $\beta^{-}$decay of ${ }_{54}^{135} \mathrm{Xe}$ (halflife $9.01 \mathrm{~h}, \lambda_{X e}=2.116 \quad 10^{-5} \mathrm{~s}^{-1}$ ) and has a peak shape, called the xenon pit. This peak may be large enough to prevent the reactor from diverging again immediately after it stops (Kerkar and Paulin 2008, p. 242), without diluting the moderator or removing the absorbing rods which generates more liquid effluents. The fission yields of ${ }_{53}^{135} \mathrm{I}$ and ${ }_{54}^{135} \mathrm{Xe}$ depend on the spectrum and the isotopic fuel composition as shown in the following Table, but an approximate value of 6\% may be used for ${ }_{53}^{135} I$ and $0.3 \%{ }_{54}^{135} \mathrm{Xe}$ in a $P W R$ of usual enrichment (around $4 \%$ in ${ }_{92}^{235} U$ ). The yields for the major fissile isotopes are given in Table 15.9 for two energy groups for more detailed calculations. There exists only the fast-group yield for isotopes that are not fissile in the thermal domains such as ${ }_{92}^{238} U$.

It can be seen that the yields of iodine 135 are almost constant for any fissile isotope whereas that of xenon 135 is very variable. This implies that the equilibrium concentration of xenon is doubled in a MOX fuel compared to UOX. ${ }^{10}$

[^325]Table 15.9 Cumulated fast and thermal yields for ${ }_{53}^{135} I$ and the independent yields of ${ }_{54}^{135} \mathrm{Xe}$ in $\%$ for the main fissile isotopes

|  | ${ }^{232}{ }_{90}^{2} \mathrm{Th}$ | ${ }_{92}^{233} U$ | ${ }_{92}^{235} U$ | ${ }_{92}^{238} U$ | ${ }_{94}^{240} \mathrm{Pu}$ | ${ }_{94}^{241} \mathrm{Pu}$ | ${ }_{94}^{242} \mathrm{Pu}$ | ${ }_{94}^{239} \mathrm{Pu}$ | ${ }_{95}^{242 m}$ Am | ${ }_{95}^{241} \mathrm{Am}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{array}{rl} \gamma_{i} & 135 \\ 53 \end{array} \text { Ithermal }<400 \mathrm{keV}_{\text {fast }}$ | 5.4328 | 4.8723 | 5.9170 | 6.5517 | 7.0314 | 7.1038 | 6.8358 | 6.5603 | 6.4314 | 5.6634 |
|  | - | 4.4065 | 6.3158 | - | - | 7.0698 | - | 6.1949 | 6.6698 | 7.0562 |
| $\gamma_{c}{ }_{54}^{135} \mathrm{Xe} e_{\text {thermal }<400 \mathrm{keV}}^{\text {fast }}>40 \mathrm{keV}$ | 0.0273 | 1.4537 | 0.4510 | 0.0167 | 0.5367 | 0.2074 | 0.0873 | 0.9651 | 0.7813 | 1.4365 |
|  | - | 1.4705 | 0.2639 | - | - | 0.2076 | - | 1.0347 | 0.7560 | 1.5764 |

### 15.10.2 Xenon Saturation

The depletion equations for one-energy group for ${ }_{54}^{135} \mathrm{Xe}$ are expressed as (Reuss 2003, p. 248; Stacey 2001, p. 213):

Bateman equations for xenon:

The capture reaction of ${ }_{53}^{135} I$ is neglected due to its weak capture cross section. $\left(\sigma^{(n, \gamma)}{ }_{2200 \mathrm{~m} / \mathrm{s}}=0.02\right.$ barns, $I^{(n, \gamma)}=0.012$ barns). ${ }^{11}$ The concentration of ${ }_{53}^{135} I$ is given by:

$$
\left[{ }_{53}^{135} I\right](t)=\left[{ }_{53}^{135} I\right](0) e^{-\lambda_{I} t}+\frac{\gamma_{I} \Sigma_{f} \Phi}{\lambda_{I}}\left(1-e^{-\lambda_{I} t}\right)
$$

The xenon concentration is calculated by writing the following:

$$
\left[{ }_{54}^{135} X e\right](t)=\alpha e^{-\lambda_{l} t}+\beta e^{-\lambda_{X_{e}} t}+\delta
$$

The initial value condition implies that $\left[{ }_{54}^{135} X e\right](0)=\alpha+\beta+\delta$. Introducing the xenon concentration in the second differential equation leads to the evaluation of $\alpha, \beta$ and $\delta$ :

$$
\begin{gathered}
-\lambda_{I} \alpha e^{-\lambda_{I} t}-\lambda_{X e} \beta e^{-\lambda_{X e} t}=\gamma_{X e} \Sigma_{f} \Phi+\lambda_{I}\left(\left[\begin{array}{c}
135 I \\
53
\end{array}\right](0) e^{-\lambda_{I} t}+\frac{\gamma_{I} \Sigma_{f} \Phi}{\lambda_{I}}\left(1-e^{-\lambda_{I} t}\right)\right) \\
-\left(\lambda_{X e}+\sigma_{X e} \Phi\right)\left(\alpha e^{-\lambda_{I} t}+\beta e^{-\lambda_{X e} t}+\delta\right) \\
\text { Hence: }\left\{\begin{array}{l}
\delta=\frac{\left(\gamma_{X e}+\gamma_{I}\right) \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi\right)} \quad \alpha=\frac{\lambda_{I}\left[{ }_{53}^{135} I\right](0)-\gamma_{I} \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi-\lambda_{I}\right)} \\
\beta=\left[{ }_{54}^{135} X e\right](0)-\frac{\lambda_{I}\left[{ }_{53}^{135} 5\right](0)-\gamma_{I} \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi-\lambda_{I}\right)}-\frac{\left(\gamma_{X e}+\gamma_{I}\right) \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi\right)}
\end{array}\right.
\end{gathered}
$$

These equations are notably simplified when considering fresh fuel, without any fission products:

[^326]\[

$$
\begin{gathered}
{\left[{ }_{53}^{135} I\right](t)=\frac{\gamma_{I} \Sigma_{f} \Phi}{\lambda_{I}}\left(1-e^{-\lambda_{I} t}\right)} \\
{\left[{ }_{54}^{135} X e\right](t)=\frac{\gamma_{I} \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi-\lambda_{I}\right)}\left(e^{-\lambda_{X_{e}} t}-e^{-\lambda_{I} t}\right)+\frac{\left(\gamma_{X_{e}}+\gamma_{I}\right) \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi\right)}\left(1-e^{-\lambda_{X_{e}} t}\right)}
\end{gathered}
$$
\]

In the case of a $U O X$ fuel enriched at $3.7 \%{ }_{92}^{235} U$, the integrated flux is approximately equal to $310^{14} \mathrm{n} / \mathrm{cm}^{2} / \mathrm{s}$, the macroscopic fission cross section around $0.037 \mathrm{~cm}^{-1}$ and the capture cross section for ${ }_{54}^{135} \mathrm{Xe}$ about 180,000 barns. Several reference works neglect the term $\lambda_{X e}\left(\begin{array}{ll}2.116 & \left.10^{-5} \mathrm{~s}^{-1}\right) \text { compared to } \sigma_{X e} \Phi\end{array}\right.$ (5.4 $10^{-5} \mathrm{~s}^{-1}$ ), and it can thus be inferred that the concentration reaches saturation point when time tends towards infinity (the asymptotic concentration being the saturated xenon):

$$
\left[{ }_{54}^{135} X e\right]^{\text {equilibrium }}=\frac{\left(\gamma_{X e}+\gamma_{I}\right) \Sigma_{f} \Phi}{\left(\lambda_{X e}+\sigma_{X e} \Phi\right)} \approx \frac{\left(\gamma_{X e}+\gamma_{I}\right) \Sigma_{f} \Phi}{\left(\sigma_{X e} \Phi\right)}=\frac{\left(\gamma_{X e}+\gamma_{I}\right) \Sigma_{f}}{\sigma_{X e}}
$$

This asymptotic concentration is independent of the flux, and thus of the power level. This simple result for a one-energy group must be clearly understood as it is valid only under the assumption that $\lambda_{X e} \ll \sigma_{X e} \Phi$, which is not really the case for $P W R$ ( $c f$. the above values in our example). Furthermore, if more precise results are required, the number of energy groups may be increased (for instance, two groups), which leads to the following equation:

$$
\left[{ }_{54}^{135} X e\right]^{\text {equilibrium }}=\frac{\left(\gamma_{X e_{1}}+\gamma_{I_{1}}\right) \Sigma_{f_{1}} \Phi_{1}+\left(\gamma_{X e_{2}}+\gamma_{I_{2}}\right) \Sigma_{f_{2}} \Phi_{2}}{\left(\lambda_{X e}+\sigma_{X e_{1}} \Phi_{1}+\sigma_{X e_{2}} \Phi_{2}\right)}
$$

thus, simplification by the flux is not possible. However, it is correct to assert that as the flux increases, the approximation is verified. It should be noted that the equilibrium iodine concentration, i.e. $\gamma_{I} \Sigma_{f} \Phi / \lambda_{I}$, varies linearly with the flux level while the equilibrium xenon concentration does not depend on the flux level as a first-order approximation, and converges towards a target concentration as shown in Fig. 15.31, whence the notion of xenon saturation. A limit to this notion of saturated xenon stems from the fact that the flux changes slowly in the assemblies during the irradiation cycle (fissile nuclides are used up and capturing fission products are formed). Numerically, 30 h are required to reach xenon saturation up to $1 \%$, i.e. a burn-up of $50 \mathrm{MWd} / \mathrm{t}$ for a 900 MWe PWR.

It may be seen from Fig. 15.31 that under the constant flux hypothesis, the amount of iodine 135 produced is directly correlated to the flux level. In the case of ${ }_{54}^{135} \mathrm{Xe}$, this effect is weaker but still observable. This phenomenon shows that the level of saturated xenon depends on the flux and that the widespread approximation of its flux independence may lead to errors of up to $40 \%$. Figure 15.32 illustrates this fact with the ratio $\left[{ }_{54}^{135} \mathrm{Xe}\right]_{0.5 \Phi \text { nominal }} /\left[{ }_{54}^{135} \mathrm{Xe}\right]_{\Phi \text { nominal }}$, and the choice of the coefficients at 0.5 and 1.5 is representative of the flux variations observed in a $P W R$. These ratios do not tend towards 1 as expected if the formula


Fig. 15.31 Xenon 135 saturation by flux level $(\times 0.5 / \times 1 / \times 1.5)$

Effet of the flux factor on the saturation of xenon 135


Fig. 15.32 Xenon 135 saturation with flux level $(\times 0.5 / \times 1.5)$ normalized to saturated xenon at nominal flux
$\left[{ }^{135} \mathrm{Xe}\right]_{\text {saturated }}=\left(\gamma_{X e}+\gamma_{I}\right) \Sigma_{f} / \sigma_{X e}$ is totally valid, thereby proving the impact of the flux on the saturation of xenon 135 .

### 15.10.3 Xenon Poisoning After Reactor Shutdown

(Rozon 1992, p. 362)
In the case of an instantaneous reactor shutdown at time $T,{ }_{54}^{135} \mathrm{Xe}$ (respectively ${ }_{53}^{135} I$ ) has an initial concentration of $\left[\begin{array}{c}135 \\ 54\end{array} \mathrm{Xe}\right](T)$ (respectively $\left[\begin{array}{c}{[135} \\ 53\end{array}\right](T)$ ) and the amount of xenon and iodine is given by:

$$
\left\{\begin{array}{l}
{\left[\begin{array}{c}
135 I \\
53
\end{array}\right](t)=\left[\begin{array}{c}
135 I \\
53
\end{array}\right](T) e^{-\lambda_{l}(t-T)}} \\
{\left[\begin{array}{c}
135 \\
\left.{ }_{54} X e\right]
\end{array}\right](t)=\left(\left[\begin{array}{c}
135 \\
\left.{ }_{54} X e\right]
\end{array}\right](T)-\frac{\lambda_{I}}{\lambda_{X e}-\lambda_{I}}\left[\begin{array}{c}
1355 \\
53
\end{array}\right](T)\right) e^{-\lambda_{X_{e}}(t-T)}+\frac{\lambda_{I}}{\lambda_{X e}-\lambda_{I}}\left[\begin{array}{c}
1355 \\
53
\end{array}\right](T) e^{-\lambda_{I}(t-T)}}
\end{array}\right.
$$

The numerical calculation shows that 22 h are required for xenon to reach its equilibrium value before the reactor shuts down. The transient ${ }_{54}^{135} \mathrm{Xe}$ is more sensitive to the initial value of ${ }_{53}^{135} I\left(\left[\begin{array}{c}135 \\ 53\end{array}\right](T)\right)$ than that of ${ }_{54}^{135} X e\left(\left[\begin{array}{c}135 \\ 54\end{array}\right] e\right](T)$ ) due to the fact that there is twice as much ${ }_{53}^{135} \mathrm{I}$ as ${ }_{54}^{135} \mathrm{Xe}$. The anti-reactivity of ${ }_{54}^{135} \mathrm{Xe}$, approximately 2700 pcm at equilibrium, reaches more than 4700 pcm at the xenon peak and hinders the divergence of the reactor if the worth of the neutron absorbers is not modified. This effect can be alleviated by reducing the power slowly and gradually, the main effect of which is to decrease the ${ }_{53}^{135} I$ concentration, which reduces the xenon peak after shutdown (Fig. 15.33).

The instantaneous nature of the reactor shutdown is a strong hypothesis which must be moderated due to the existence of delayed neutrons that induce fission reactions (thereby increasing xenon and iodine production momentarily), and furthermore, the assemblies in the core are not all subject to the nominal flux. Indeed, the peak level and the time at which it occurs depend on the iodine level reached before shutdown. This is also valid if the reactor power is decreased before shutdown. Figure 15.34 illustrates the effect of the power level before shutdown on the occurrence of the xenon peak, which varies by up to $\pm 2 \mathrm{~h}$ with respect to the shutdown calculation after irradiation under nominal flux.

The "reactor shutdown" situation also occurs during the load-following sequence where the reactor power varies with steps and can cause time oscillations of the ${ }_{54}^{135} \mathrm{Xe}$ concentration.


Fig. 15.33 Iodine 135 and xenon 135 transients following instantaneous reactor shutdown after 200 operating hours at nominal power


Fig. 15.34 Power level effect on the xenon peak before shutdown

### 15.11 Samarium Physics

${ }_{62}^{149} \mathrm{Sm}$ is a stable samarium isotope that is produced in very small quantities by fission and mostly by the decay of ${ }_{61}^{149} \mathrm{Pm}$ with a 53-h half-life (Fig. 15.35 provides the order of magnitude of the fission yields and the two-group capture crosssections). This isotope is the sixth most absorbing fission product after ${ }_{54}^{135} \mathrm{Xe}$ (Reuss 2003, p. 246) and causes an anti-reactivity effect of about 700 pcm at its saturated concentration in a burnt fuel.

It should be carefully noted that promethium 148 cross sections have varied significantly over the years. The thermal cross section of this isotope decreased tenfold between the SERMA79 evaluation (cf. the previous edition of this work) and the JEFF3 evaluation. Detailed analysis has shown that this isotope varies significantly between each evaluation, proving that it is not well-known despite its importance in the samarium 149 chain. Using the cross-section values, it can be seen that $99.6 \%$ of samarium 149 production emanates from the decay of promethium 149 , and the rest from the capture of samarium $148 .{ }^{12}$ When the reactor is shut down, ${ }_{61}^{149} \mathrm{Pm}$, with a concentration almost half of that of samarium, decays to ${ }_{62}^{149} \mathrm{Sm}$ that does not disappear under flux (Fig. 15.36) (Reuss 2003, p. 252; Stacey 2001, p. 210), and hinders the restart of the reactor just like xenon, though to a lesser extent due to its lower absorption.

However, unlike ${ }_{54}^{135} \mathrm{Xe}$ which is radioactive, the stable samarium produced during the shutdown period does not disappear. From operating experience from the nuclear reactor fleet, it is shown that the critical boron concentration is overestimated by 30 ppm if this effect is neglected.

Unlike ${ }_{54}^{135} \mathrm{Xe},{ }_{62}^{149} \mathrm{Sm}$ is never completely saturated in the fuel and its concentration increases significantly during burn-up due to the variation of cross sections by

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Fig. 15.35 Decay/capture scheme of samarium 149 (JEFF3 data for UOX 3.7\% at 20,000 MWd/t on)


Fig. 15.36 Evolution of samarium concentration after reactor shutdown
spectral effects, and is weakly dependent on the flux. However, the concentration of ${ }_{61}^{149} \mathrm{Pm}$ is almost proportional to the flux and is greatly impacted by a stretch-out.

### 15.12 Gadolinium Physics

Gadolinium is a particularly efficient neutron absorber, similar to several rare earths (hafnium and erbium, which are also used in the nuclear industry). It was discovered in 1886 as gadolinium oxide by Mérignac and Lecoq de Boisbaudian. It is a metal with a relative (to water) density of 7.868 that is mixed homogeneously (although not perfectly) with the fuel in its oxide form, $\mathrm{Gd}_{2} \mathrm{O}_{3}{ }^{13}$ However, natural

[^328]

Fig. 15.37 Gadolinium capture chain with the natural isotopic abundance and the resonance integral
gadolinium contains several isotopes including those of odd mass numbers $\left({ }_{64}^{155} G d\right.$ and ${ }_{64}^{157} G d$ ) that are highly absorbing. ${ }^{14}$ Increasing the natural cycle length is carried out by increasing the initial enrichment of assemblies. For safety reasons (boron crystallization, negative moderator temperature feedback coefficient), the critical boron concentration in water, allowing the core to become critical at start-up, cannot be increased too much, nor can the assembly be enriched (peaking factor). One solution to this problem consists in poisoning certain assemblies with gadolinium, which is a burnable absorber given that the odd isotopes disappear during the cycle, and thus the core reactivity increases (gadolinium oxide content of $10 \%$, mixed with uranium oxide). The major advantage of gadolinium is that it is used up progressively, thus allowing a reactivity increase of around $20,000 \mathrm{MWd} / \mathrm{t}$ for the infinite lattice case. Further, it meets several technological requirements: good mechanical behavior, chemical stability, good thermal conductivity, easily recycled, no significant reduction of power density, readily available and easily managed (Fig. 15.37).

A suitable calculation scheme should allow for the effect of gadolinium on assembly reactivity. ${ }^{15}$

### 15.13 The Industrial Fuel Cycle in France

(Jurain 1964)
The fuel cycle corresponds to the life cycle of nuclear matter that will be discussed later to define the terms employed. It may be said that the nuclear fuel is "born" at the mine and "dies" diluted in acid during recycling at the plant in The Hague (AREVA NC). Some of its most "noble" components such as uranium and plutonium may be used again to manufacture a new fuel: thus, there is a closed fuel cycle (Fig. 15.38):

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Fig. 15.38 Schematic representation of the French fuel cycle (http://www.french-nuclear-safety. fr/ASN/About-ASN/Activities-monitored-by-ASN/Waste-decommissioned-facilities)

The French fuel cycle has a specific feature, shared by the Belgian cycle, whereby plutonium can be significantly recycled through the manufacture of $M O X$ assemblies (for Mixed Oxide) with both $\mathrm{UO}_{2}$ and $\mathrm{PuO}_{2}$. Initially, the goal of recycling was to provide pure and high-grade plutonium (almost pure ${ }_{94}^{239} \mathrm{Pu}$ ) for the manufacture of the first French atomic bombs, since bombs with pure ${ }_{92}^{235} U$ required costly technological investment with no guarantee of success during the post-war period in France [gas diffusion technology is complex and required high investment; for more information, see (Goldschmidt 1987)]. At the end of the 1970s, it was decided to recycle plutonium in a fleet of fast neutron reactors, such as SUPERPHENIX, which are breeder reactors in plutonium with the use of "fertile blankets" (rows of assemblies with pure ${ }_{92}^{238} U$ ). The oil crisis was at its height, and plutonium was seen as an energy raw material that could be immediately employed. Today, the context is different, and observations no longer as clear-cut, with plutonium stocks being considered at times as an inconvenient nuclear waste. It is used partially in French $P W R$ today (unlike the US strategy for example) but second-generation plutonium (from the possible recycling of $M O X$ ) is poor in ${ }_{94}^{239} P$ $u$ and not very suitable for recycling since the plutonium content must be increased above the limits set by the safety studies at present (about $12 \%$ of plutonium in an assembly). Thus, a mixing technique with materials having higher plutonium contents is required. Indeed plutonium recycling is not very intensively performed, since only 900 MWe reactors are allowed to load such assemblies at present, resulting in only a very slight reduction in the plutonium stock. Debates often
arise between pro- and anti-recycling supporters, and at times MOX fuel processing itself is criticized. Solutions involving storage of entire assemblies at the end of life (dry storage) have even been considered, but the subject of nuclear waste continues to be a societal issue in itself.

Natural uranium is obtained from the uppermost 10 km of the Earth crust, but small quantities are also present in sea water (about $3 \mathrm{mg} /$ ton of water), thereby making the oceans a huge uranium reservoir if an economically viable means of extraction can be found. On land, uranium is obtained from Canada, the United States, South Africa, Australia, Nigeria and Gabon. France does not have a significant uranium reserve, although in the past, uranium mines existed in the regions of Lodève and Coutras. In Canada, the Cigar Lake mine contains ore with an exceptionally high content of $12 \%$. By comparison, ore from the open-air Arlit mine in Niger, discovered in 1966 by the French, has a 5\% uranium content.

Uranium is produced by the enrichment process as sodium diuranate (yellow cake containing $75 \%$ uranium). It should be noted that 165 tons of concentrated uranium are required for a single equilibrium load of a 1000 MWe reactor (with the fuel enriched at $3.1 \%$ in ${ }_{92}^{235} U$ ). Uranium is then processed by the conversion factory where the yellow cake $\left(U_{3} O_{8}\right)$ is transformed to uranium hexafluoride, $U F_{6}$, (this conversion is also called fluorination). France uses the wet process, which comprises the following steps:

- dissolution of the concentrates in nitric acid,
- purification of uranyl nitrate using an extraction process with tributyl phosphate (TBP),
- Precipitation of ammonium diuranate (ADU),
- Calcination to produce $\mathrm{UO}_{3}$, which when reduced produces $U O_{2}$,
- Hyper-fluorination of $U O_{2}$ to solid $U F_{4}$,
- Fluorination of $U F_{4}$ to $U F_{6}$. Recycled uranium may be fluorinated, although this is expensive due to the initial radioactivity.

Uranium enrichment is required only for water reactors. Indeed, light water is an excellent moderator but has a relatively non-negligible capture cross-section. Thus, natural uranium must be enriched with the fissile isotope ${ }_{92}^{235} U$, in contrast with the UNGG (Natural Uranium Graphite Gas reactors, the first French reactor) reactor, in which the moderator comprised graphite blocks, allowing natural uranium to be used. In practice, the UNGG reactor was slightly enriched to increase the cycle length for economic considerations. To obtain a critical pin lattice in $P W R$ while meeting the thermal-hydraulic cooling constraints, a target enrichment value of $4 \%$ ${ }_{92}^{235} U$ is required (Fig. 15.39).

Starting with 165 tons of concentrated uranium as gaseous $U F_{6}$ and assuming depleted enrichment of $0.25 \%$ (uranium depleted by the enrichment process), 27 tons of enriched uranium at $3.1 \%$ are needed to produce one loading pattern of assemblies (cf. Fig. 15.40). This enrichment requires 108000 separative work units ( $S W U$ ). At room temperature $U F_{6}$ is a colorless crystalline solid; it sublimates at $56{ }^{\circ} \mathrm{C}$ and at 1 bar , making it an excellent vector in the enrichment process. The


Fig. 15.39 Transformation of 1 kg of natural uranium for one UOX $3.25 \%$ fuel management cycle (one-third core, unloaded at $33,000 \mathrm{MWd} / \mathrm{t}$ )
principle of gaseous diffusion is based on Graham's law of effusion, which demonstrates that if molecules of a gas of mass $m$ with Boltzmann speed distribution are placed in a box, and a hole is made in surface $S$ at the bottom of the box, the time variation of the number of molecules due to leakage through the hole is inversely proportional to the square root of the mass of that molecule:

$$
\begin{equation*}
\text { Graham's law: } \frac{d N}{d t}=N S \sqrt{\frac{k T}{2 \pi m}} \tag{15.11}
\end{equation*}
$$

The process thus relies on the diffusion of gaseous $U F_{6}$ through a porous membrane called a barrier. The pores are of very small radius ( $<200$ angstroms) and the material comprising the barrier must be as permeable as possible. Lighter nuclides pass through the barrier preferentially, unlike the heavier ones. Gradual enrichment thus occurs in ${ }_{92}^{235} U$ and also in ${ }_{92}^{234} U$, which can reach a content of 400 ppm . In industrial settings, several enrichment loops are created in series and the residue from step $N$ is injected towards $N-1$, while the concentrate from step $N$ goes to step $N+1$. This is called a diffusion cascade (Murray 1954, p. 68). The energy required for the compressors makes the process very costly. In France, the Georges Besse plant operated by Eurodif employs this process. To give an idea of the energy consumption this plant, it is often said that it uses the entire production of a reactor from the neighboring Tricastin site.

The Georges Besse 2 enrichment plant (started in 2011), utilizes a different enrichment principle, ultra-centrifugation, based on centrifugal force to separate more heavy nuclei from lighter nuclei. If a container of gaseous $U F_{6}$ is rotated very rapidly, over-concentration of heavy nuclides occurs at the outer sections of the


Fig. 15.40 NUMEC (1966) enrichment calculation rule: This calculation cardboard indicates the mass (in kg ) of SWU (UTS in French) and of natural uranium (at $0.711 \%$ ) needed for a given enrichment (in this example, $3.70 \%$ ) with an imposed enrichment tail (for a tail waste value of $0.22 \%$, see column 7 , the value of SWU is 5.584 kg and that of natural uranium 7.088 kg ). The first side of the table gives the results for a rejected enrichment within the $0.10-0.28 \%$ range, and the other side for the $0.30-0.65 \%$ range. It can be seen that the table provides values up to military enrichments of $95 \%$ in uranium 235! For a target enrichment of $3.10 \%, 6.217 \mathrm{~kg}$ of natural uranium with a rejected enrichment of $0.2531 \%$ are required, which for 27 tons of enriched uranium, indicates 167 tons of natural uranium to be enriched, thereby corroborating the values given in the text, with the residual discrepancy ( 165 tons) being due to the small difference in rejected enrichment. (The Marguet collection)
centrifuge (namely ${ }_{92}^{238} U$ ). This process is around 20 times less expensive than gaseous diffusion but poses complex technological problems concerning the stability and the design of the plateaus owing to the high rotation speed (around 50,000 rpm!). Other enrichment processes exist at the laboratory test stage, including selective excitation
of uranium vapor by emission of a laser wave at the same specific wavelength as ${ }_{92}^{235} U$. The resulting ionization enables the separation of ${ }_{92}^{235} U$ from ${ }_{92}^{238} U$ ions by applying a magnetic field (their paths are different and they are recovered separately). This laser procedure is highly selective ${ }^{16}$ in theory (less than $1{ }_{92}^{238} U$ parasite ions for over $10,000{ }_{92}^{235} U$ ions!), thereby making it highly proliferative, which accounts for the confidential nature of such advanced technologies.

The enrichment process is followed by the manufacture of fuel assemblies. A $P W R$ (the most widely used technology in France) assembly contains 264 fuel pins and 25 guide thimbles for inserting absorbing control rods. The lattice pitch is 12.6 mm . The manufacturing plant transforms uranium hexafluoride $U F_{6}$ into uranium dioxide $\mathrm{UO}_{2}$. The oxide is then formed by sintering into fuel pellets with a diameter of 8.2 mm , which are placed in Zircaloy tubes. An assembly for a 900 MWe reactor contains 461.4 kg of uranium metal (not to be confused with the mass of the oxide, $\mathrm{UO}_{2}$, or with the mass of the entire assembly, which is 649 kg for a height of 4.058 m , with 3.66 m of active height, i.e. the fuel height). An assembly for a 1300 MWe reactor is higher ( 4.796 m , with an active height of 4.267 m ) and has a uranium metal weight of 538.8 kg (the total assembly mass is 760 kg , of which 610.8 kg of $\mathrm{UO}_{2}$ ). These assemblies make up the core loading pattern. 34.5 ton of uranium enriched at $3.1 \%$ are required to manufacture the loading pattern of 64 assemblies for 1300 MWe reactors with one-third core fuel management (short cycle). These reactors contain 104 ton of uranium dioxide. The fuel is placed, in the form of pellets, in a cladding tube made of Zircaloy 4 (an alloy consisting mainly of zirconium). The fuel is changed every 3 or 4 years ( 52 assemblies with one-third core fuel management for a 900 MWe reactor or 64 assemblies for 1300 MWe reactor). The current strategy is to design longer fuel cycles by increasing fuel enrichment so as to optimize fuel use-up (Kerkar and Paulin 2008).

Generally speaking, for economic reasons, fuel management systems are becoming increasingly complex, in terms of both fuel diversity and fractioning of the loading pattern. After its life in the reactor, the irradiated fuel is cooled in a fuel pool before being transferred to a recycling plant (La Hague in France). Today, recycling enables retrieval of fissile plutonium that can be used as a "raw material" for fast neutron reactors or $M O X$ fuel. Furthermore, recycling is also a safe means of treating high-activity nuclear wastes (fission products), and it thus helps to decrease the amounts to be stocked. After a minimum of 8 months of cooling (required to attain a residual power of less than 8 kW ), the irradiated fuel assemblies are transferred to fuel casks, which can contain up to 12 assemblies (e.g. TN12 type) and transported to the AREVA NC plant in La Hague.

The assemblies are then sheared and immersed in a rotating solvent containing concentrated nitric acid ( 4 to 10 times the normal concentration). The fission products are extracted using a solvent (tributyl phosphate or TBP) and then decanted. This process is called the co-decontamination phase. Uranium and

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Fig. 15.41 A proposed gallery network for sub-surface storage ( 50 m below ground level, Andra)
plutonium are separated via a second extraction cycle (counter-flow solvent in a reductive aqueous phase). This is followed by a uranium purification cycle to reduce the remaining traces of plutonium. The recycled uranium contains traces of ${ }_{92}^{232} U$ that can lead to radioactivity problems, as well as a large quantity of ${ }_{92}^{236} U$, which is a neutron absorber, making Enriched Reprocessed Uranium (ERU) more difficult to use.

Active wastes at all levels of fuel recycling must be stocked. Storage of nuclear waste is very complex: how can nuclear wastes be stored safely for thousands of years, the time needed for radioactive decay to fall to within acceptable levels? The deep disposal solution of is one of the most viable currently being considered. Nevertheless, long-term deep disposal poses security problems such as inappropriate water intrusion (loss of barriers and lixiviation of materials) as well as unwanted mechanical intrusion (human). Reversible storage strategies (with the possibility of future recycling of wastes by keeping them at an accessible location) have also been studied. Confinement (such as sealing of waste wells, waste recycling, etc.) is more critical since this strategy, by definition, implies more difficult access to nuclear waste materials (Fig. 15.41).

## Chapter 16 Neutronic Feedback

Understanding the effect on neutronics of the changing physical parameters of a pile is a key element in safety analysis. These effects are known as "neutron feedback" and have various and complex origins. In industrial reactors, a high moderator temperature is required either to vaporize water or to increase the thermal efficiency of the reactor. This high temperature implies significant fluctuations in the fuel temperature, which in turn affects cross sections via the Doppler effect. Furthermore, the moderator density also varies significantly, thereby influencing neutron slowing-down.
(Hummel and Okrent 1970) for fast-neutron reactors, (Reuss 2003, p. 277) for PWR

### 16.1 Effect of Fuel Temperature on the Multiplication Factor

### 16.1.1 Fuel Doppler Effect

(Hummel and Okrent 1970, p. 133; Silvennoinen 1976, p. 77; Meghreblian and Holmes 1960, p. 308)

Let the expression of the effective multiplication factor be: $k_{e f f}=k_{\infty} P_{n f}=\eta \varepsilon p f P_{n f}$ where $P_{n f}$ is the non-leakage probability of the finite reactor ( $P_{n f}=e^{-B_{g}^{2} \tau_{t h}} /\left(1+L^{2} B_{g}^{2}\right)$ according to Fermi's age theory). Deriving this expression logarithmically:

$$
\alpha_{D}=\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T}=\frac{1}{\eta} \frac{\partial \eta}{\partial T}+\frac{1}{\varepsilon} \frac{\partial \varepsilon}{\partial T}+\frac{1}{p} \frac{\partial p}{\partial T}+\frac{1}{f} \frac{\partial f}{\partial T}+\frac{1}{P_{n f}} \frac{\partial P_{n f}}{\partial T}
$$

$\alpha_{D}$ is called the Doppler coefficient. The reactivity effect $\rho=\frac{k_{\text {eff }}-1}{k_{\text {eff }}}$ is given by:

$$
\frac{\partial \rho}{\partial T}=\frac{1}{k_{e f f}{ }^{2}} \frac{\partial k_{e f f}}{\partial T}=\frac{1}{k_{e f f}}\left(\frac{1}{\eta} \frac{\partial \eta}{\partial T}+\frac{1}{\varepsilon} \frac{\partial \varepsilon}{\partial T}+\frac{1}{p} \frac{\partial p}{\partial T}+\frac{1}{f} \frac{\partial f}{\partial T}+\frac{1}{P_{n f}} \frac{\partial P_{n f}}{\partial T}\right)
$$

The predominant term in this expression is due to the contribution of the resonance escape probability $\partial p /(p \partial T)$. The latter is significantly impacted by the Doppler effect, which causes increased capture in the fuel resonances (especially for ${ }_{92}^{238} U$ ). This resonance escape probability is written as:

$$
\begin{aligned}
p & =e^{-\frac{I_{e f f} N_{U}}{\xi \Sigma_{c}} N_{\mathrm{mod}}} \\
\alpha_{D} & \approx \ln (p) \frac{1}{I_{e f f}} \frac{\partial I_{\text {eff }}}{\partial T}
\end{aligned}
$$

The relative change in $I_{\text {eff }}$ is sometimes called the Doppler efficiency. In the Narrow Resonance-Infinite Mass (NRIM) approximation, the resonance integral at energy $E_{0}$ is written as:

$$
I_{\gamma}=\frac{\sigma_{0} \Gamma_{\gamma}}{E_{0}} \beta J(\xi, \beta)
$$

where $J(\xi, \beta)$ is the Dresner function, seen in Chap. 6, and $\beta=\left(\sigma_{m}+\sigma_{e}\right) \Gamma /\left(\sigma_{0} \Gamma_{\gamma}\right)$. It will be recalled that where the dilution cross section $\sigma_{m}$ tends to infinity, $\beta J(\xi, \beta)$ tends towards $\pi / 2$. The Doppler effect widens the resonances when the target nuclei temperature increases. Furthermore, it should be noted that a (capture) cross section may be modeled using the Breit-Wigner formalism with the Voigt function $\psi$ :

$$
\bar{\sigma} \approx \sigma_{0} \frac{\Gamma_{i}}{\Gamma} \Psi(x, \xi)=\sigma_{0} \frac{\Gamma_{i}}{\Gamma}\left[\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{e^{-\frac{\xi^{2}}{4}(y-x)^{2}}}{y^{2}+1} d y\right]
$$

The capture cross sections are more sensitive to temperature than the diffusion cross sections and we will thus focus on this reaction cross section. Usually, the area bounded by the cross section resonance is independent of temperature:

$$
A(T)=\int_{-\infty}^{+\infty} \bar{\sigma}(x, T) d E=\frac{\pi}{2} \sigma_{0} \Gamma_{i}
$$

Therefore, if the resonance peak decreases, the latter widens because of the Doppler effect. Actually, due to the self-shielding process for an absorbing material and the fact that $\sigma_{0}$ is not strictly constant, the area under the Voigt plot depends slightly on temperature. To compute the absorption rate of this resonant cross


Fig. 16.1 Resonance effect on flux and reaction rate
section, it is assumed as a first approximation that the resonance is a "black trap" of width $\Delta$, from which no neutrons can escape. Therefore, as $\Delta$ increases with temperature, so too does the absorption rate. In real-life physics, the trap is said to be "grey", but the flux is less depressed in the resonance, which is flattened by the Doppler effect. In the end, the absorption rate increases, hence decreasing reactivity. Figure 16.1 illustrates the fact that the product of the average cross section and the average flux ( $\bar{\Phi}$ for cold and $\bar{\Phi}$ for hot) in the trap (i.e. the average reaction rate) is higher for the hot case (red line) than for the cold case (in blue).

The problem may be simplified by considering a cross section with a continuous background value of $\sigma_{p}$ out of the resonance of width $\Delta$ for the cold case and $\delta \Delta$ for the hot one $(\delta>1)$. Given that the effective cross section integral is conserved, the peak value of the cross section falls to $\sigma_{0, \gamma} / \delta$ for the hot temperature. Since the flux is inversely proportional to $\sigma_{t},{ }^{1}$ the respective microscopic capture rates in both situations are:

$$
R_{\text {cold }}=\frac{\sigma_{0, \gamma}}{\sigma_{0, \gamma}+\sigma_{p}} \Delta \quad \text { and } \quad R_{h o t}=\frac{\frac{\sigma_{0, \gamma}}{\delta}}{\frac{\sigma_{0, \gamma}}{\delta}+\sigma_{p}} \delta \Delta
$$

Hence:

$$
\frac{R_{\text {hot }}}{R_{\text {cold }}}=\frac{\delta\left(\sigma_{0, \gamma}+\sigma_{p}\right)}{\sigma_{0, \gamma}+\delta \sigma_{p}}>1
$$

Even though the cross section integral is conserved, the capture rate increases by self-shielding. Defining the mean values of the cross section and the flux in a resonance, therefore:

[^331]

Fig. 16.2 Comparison of the spectra for a Fast Neutron Reactor (SuperPhenix), a MOX PWR, and a UOX PWR. The resonance effect leads to localized depressions in the flux. The MOX spectrum is harder than that of the UOX case. The Maxwell distribution of the MOX fuel is severely perturbed by the plutonium isotope resonances. Normalized flux, RNR teneur $14 \%=\operatorname{SFR}(1200 \mathrm{MWe})$ Pu content $14 \%$, REP-MOX teneur $5.3 \%=$ MOX PWR ( 900 MWe ) Pu content $5.30 \%$, REP-UOX enrichissement $3.25 \%$ = UOX PWR ( 900 MWe) enrichment $3.25 \%$

$$
\begin{aligned}
\int \sigma\left(E, T_{\text {cold }}\right) \Phi\left(E, T_{\text {cold }}\right) d E & \approx \overline{\sigma\left(T_{\text {cold }}\right)} \overline{\Phi\left(T_{\text {cold }}\right)} \Delta \leq \overline{\sigma\left(T_{\text {hot })}\right.} \overline{\Phi\left(T_{\text {hot }}\right)} \delta \Delta \\
& \approx \int \sigma\left(E, T_{\text {hot }}\right) \Phi\left(E, T_{\text {hot }}\right) d E
\end{aligned}
$$

The same reasoning may be applied for the fission rate. Finally, the Doppler effect depends on the balance between capture and fission. In a uranium fuel, capture on ${ }_{92}^{238} U$ prevails and the effect is stabilizing (Fig. 16.2 shows the hardening effect of resonance on flux spectrum for different fuels).

### 16.1.2 Doppler Effect on Reactor Behavior

The increase in the absorption rate induces a negative effect on reactivity $\left(\partial k_{\text {eff }} \partial T_{\text {fuel }}<0\right) .{ }^{2}$ This is a stabilizing effect in the event of a power excursion.

[^332]Indeed, in such a situation, this effect leads to a fast rise in the fuel temperature, which is even faster if the fuel is cold. It is the fastest effect and takes place within seconds of the sudden increase in power, especially for oxide fuel, owing to the poor thermal conductivity of oxides compared to metals. The Doppler effect is in fact characterized by:

- an increase in the resonance integral with temperature,
- an increase in the resonance escape probability $p$,
- a decrease in $k_{\infty}$.

For instance, the mean change over an entire $P W R$ (moderating ratio of 1.95) is: $\Delta k / k \approx-1.8 \mathrm{pcm} /{ }^{\circ} \mathrm{C}$. In the example above, with a mean fuel temperature of $600{ }^{\circ} \mathrm{C}$, about 1000 pcm are lost during the power rise. The Doppler effect is an important factor for the stability of uranium-oxide reactors in the event of a power excursion:

- It occurs immediately, before the moderator temperature coefficient, which occurs later,
- Since uranium oxide is a poor heat conductor, its temperature rises quickly to high values in the central part of the pins (more than $2000{ }^{\circ} \mathrm{C}$ ): reactivity decreases even more for pins that are more enriched, which undergo the most significant decrease in specific power,
- The Doppler effect always acts as a stabilizer to counteract temperature increase. This is not the case for the void effect, which may change signs depending on the geometry and the fuel loaded.

If we compare the Doppler effects for three different fuel types, $4.2 \%$ UOX, $3.2 \% \mathrm{MOXI}^{3}$ and $7.8 \%$ MOX3, computed in an infinite lattice with a geometric moderating ratio of 1.66 (under-moderated), Plutonium build-up in the UOX assembly with burn-up tends to increase the differential Doppler. Over the cycle, the $U O X$ behaves more like a $M O X$ fuel as plutonium appears, and the hardening of the spectrum promotes epithermal captures in ${ }_{92}^{238} U$. Regarding $M O X$, the spectrum is already hard. However, the decrease over the cycle causes a decrease in the differential Doppler coefficient. Furthermore, MOX Pu content has a relatively slight effect for a given isotopic composition (Fig. 16.3).

[^333]

Fig. 16.3 Reactivity effect for the differential Doppler effects for 3 fuel types in an undermoderated lattice for a rise of $254{ }^{\circ} \mathrm{C}$ (cold case at $286{ }^{\circ} \mathrm{C}$, hot case at $540{ }^{\circ} \mathrm{C}$ )

### 16.2 Moderator Temperature Effect

### 16.2.1 Definitions

The effect of moderator temperature on reactivity is varied and complex (Glasstone and Sesonske 1994, p. 276). If the water (moderator) temperature increases in a PWR, the density decreases (if $N_{\text {mod }}$ is the moderator concentration, $d N_{\text {mod }} / d T_{\text {mod }}=$ $-\beta N_{\text {mod }}$ where $\beta$ is the thermal-expansion volume coefficient). Hence, moderation is less effective and the spectrum "hardens" (shift towards the epithermal range). The fission cross sections decrease. This effect is anti-reactive but it should be pointed out that some capture cross sections with a $1 / v$ tendency also decrease. This effect is slightly counterbalanced by the decrease in the number of boron nuclei diluted in water, which reduces the absorption rate. The amount of boron depends on the operating point of the reactor. There is also a Doppler effect on the cross sections of the isotopes in the water molecule (hydrogen and oxygen), especially for the high-energy resonances of the scattering cross section of oxygen. In the end, the total effect is negative for a PWR $\left(\partial k_{\text {eff }} \partial T_{m}<0\right)$ since the major effect is a decrease in moderation as temperature increases. A typical order of magnitude is $\partial k_{\text {eff }} / \partial T_{m} \approx-40 \mathrm{pcm} / \mathrm{K}$. The moderator temperature coefficient (MTC) is usually given as:

$$
\alpha_{m} \equiv \frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T_{m}}
$$

Although in strict terms, this equation is defined locally in the reactor, in practice, an average temperature is used. The moderator density effects (change in density at constant temperature) on the water cross sections are distinguished from the temperature effects (Doppler effect). Assuming that $k_{\text {eff }}$ depends on $\rho_{m}$ and $T_{m}$ :

$$
d k_{e f f}=\left.\frac{\partial k_{e f f}}{\partial \rho_{m}}\right|_{T_{m}} d \rho_{m}+\left.\frac{\partial k_{e f f}}{\partial T_{m}}\right|_{\rho_{m}} d T_{m}
$$

Thus: $\quad \alpha_{m}=\frac{1}{k_{e f f}}\left(\left.\frac{\partial k_{e f f}}{\partial \rho_{m}}\right|_{T_{m}} \frac{d \rho_{m}}{d T_{m}}+\left.\frac{\partial k_{e f f}}{\partial T_{m}}\right|_{\rho_{m}}\right)=\alpha_{\rho_{m}} \frac{d \rho_{m}}{d T_{m}}+\alpha_{T_{m}}$
This equation defines the isothermal density coefficient $\alpha_{\rho_{m}}$, which is the relative change in $k_{\text {eff }}$ for a moderator density change. It takes into account the change in the moderating ratio as moderator density changes. The constant-density moderator temperature coefficient $\alpha_{T_{m}}$, also called the constant-density spectral coefficient, is the relative change in $k_{\text {eff }}$ for a change in moderator density under prescribed density conditions. It allows for the Doppler effect on the moderator cross sections. It is also an indicator of the change in target nuclei kinetic energy. It may be seen that for a two-phase moderator, density and temperature are no longer implicitly correlated due to the presence of an average void fraction, denoted $\bar{u}$. The void coefficient is defined as:

$$
\alpha_{v} \equiv \frac{1}{k_{\text {eff }}} \frac{\partial k_{\text {eff }}}{\partial \bar{u}} \approx \frac{1}{k_{\text {eff }}} \frac{\delta k_{\text {eff }}}{\delta \rho_{m}} \frac{\delta \rho_{m}}{\delta \bar{u}}=\alpha_{\rho_{m}} \frac{\delta \rho_{m}}{\delta \bar{u}}
$$

Similarly, the pressure coefficient is equal to:

$$
\alpha_{p} \equiv \frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial p} \approx \frac{1}{k_{e f f}} \frac{\delta k_{e f f}}{\delta \rho_{m}} \frac{\delta \rho_{m}}{\delta p}=\alpha_{\rho} \frac{\delta \rho_{m}}{\delta p}
$$

These formulae show that all differential coefficients may be expressed in terms of $\alpha_{\rho_{m}}$ and $\alpha_{T_{m}}$. The most commonly used coefficient is the moderator alpha coefficient, which links change in reactivity to the moderator temperature:

$$
\Delta \rho=\rho-\rho_{r e f}=\alpha_{\bmod }\left(T_{m}-T_{m}^{r e f}\right)
$$

Mathematically, by the definition of reactivity $\rho \equiv\left(k_{\text {eff }}-1\right) / k_{\text {eff }}$ itself:

$$
\alpha_{\mathrm{mod}}=\frac{\delta \rho}{\delta T_{m}}=\frac{1}{k_{\text {eff }}^{2}} \frac{\partial k_{e f f}}{\partial T_{m}}=\frac{1}{k_{e f f}} \alpha_{m} \approx \alpha_{m} \quad \text { close to criticality }
$$

The moderator alpha coefficient is negative in this form and is expressed in $p \mathrm{~cm} /{ }^{\circ} \mathrm{C}$. In one-group theory, the following may be written:

$$
\Delta \rho \equiv \rho-\rho_{r e f}=\left(1-\frac{1}{k_{e f f}}\right)-\left(1-\frac{1}{k_{e f f}^{r e f}}\right)
$$

Fig. 16.4 Effect of moderating ratio on reactivity


Disregarding leakage effects, $\Delta \rho \approx \Sigma_{a}^{r e f} / v \Sigma_{f}^{r e f}-\Sigma_{a} / v \Sigma_{f}$. Assuming that at first order, only the absorption cross section changes under the influence of the moderator, $\Delta \rho \approx-\Delta \Sigma_{a} / v \Sigma_{f}$ where $\Delta \Sigma_{a} \approx-v \Sigma_{f} \alpha_{\bmod }\left(T_{\bmod }-T_{\bmod }^{r e f}\right)$. The specific moderating ratio, that is the ratio of the moderator nuclei to fuel nuclei, is a very useful notion.

The moderating ratio $\rho_{m} V_{m} / \rho_{U} V_{U}$ may vary because of expansion effects; in particular, for a $P W R$ with a liquid-phase moderator, the number of moderator nuclei $N_{m} V_{m}$ decreases as the temperature rises. The moderator has two opposite properties: it slows down neutrons (affecting the resonance escape probability $p$ ) and it has a varying absorbing capability (affecting the thermal utilization factor $f$ ) (Fig. 16.4).

The term technological moderating ratio is used in the industrial world and is defined as the volume ratio between moderator and fuel. The optimum value for a $P W R$ is around 4 (Reuss 2003, p. 231). An under-moderated reactor operating to the left of the maximum is stable in the event of a temperature rise with a decrease in the moderating ratio-this effect reduces $k_{\infty}$. On the other hand, a reactor operating to the right of the maximum value is unstable if the temperature rises with a decrease in the moderating ratio. All modern $P W R$ are under-moderated by design and must remain so during operation to ensure a negative temperature coefficient, as prescribed by safety regulations. This limits the amount of boron used as a soluble absorber.

### 16.2.2 Leakage and Absorber Effects

The reactivity of a reactor may be modeled to account for the absorption of rods and soluble poisons (capture term $C<1$ ), as well as for neutron leakage (characterized by fast and thermal non-leakage probabilities, i.e. $\left.F=\left(1-P_{r}\right)\left(1-P_{t h}\right)<1\right)$. Therefore:

$$
k_{e f f}=k_{\infty} F C
$$

Using these notations and logarithmic derivation, the isothermal density coefficient is written as:

$$
\left.\alpha_{\rho_{m}} \equiv \frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial \rho_{m}}\right|_{T_{m}}=\left.\frac{1}{k_{\infty}} \frac{\partial k_{\infty}}{\partial \rho_{m}}\right|_{T_{m}}+\left.\frac{1}{F} \frac{\partial F}{\partial \rho_{m}}\right|_{T_{m}}+\left.\frac{1}{C} \frac{\partial C}{\partial \rho_{m}}\right|_{T_{m}}
$$

We have just seen that the first coefficient has an optimum value with the moderating ratio. Indeed, a high moderating ratio decreases the thermal utilization factor while a low one increases the epithermal and fast absorption probability in solid materials. The former coefficient is positive under PWR operating conditions at nominal power since the moderating ratio is to the left of the maximum value (such that a decrease or void density lowers reactivity). Since $d \rho_{m} / d T_{m}$ is negative under one-phase (water) conditions, the contribution of the first term to MTC is negative:

$$
\left.\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial \rho_{m}}\right|_{T_{m}} \frac{\partial \rho_{m}}{\partial T_{m}}<0
$$

Using the age theory to model leakage $\left(1-P_{r}\right)=e^{-B_{g}^{2} \tau_{t h}}$ :

$$
F=\frac{1}{1+M^{2} B_{g}^{2}}=\frac{e^{-B_{g}^{2} \tau_{t h}}}{\left(1+L^{2} B_{g}^{2}\right)} \approx \frac{1}{\left(1+\tau_{t h} B_{g}^{2}\right)\left(1+L^{2} B_{g}^{2}\right)}
$$

Differential leakage effect may be computed:
$\left.\frac{1}{F} \frac{\partial F}{\partial \rho_{m}}\right|_{T_{m}}=-\frac{1}{\left(1+\tau_{t h} B_{g}^{2}\right)}\left(B_{g}^{2} \frac{\partial \tau}{\partial \rho_{m}}+\tau \frac{\partial B_{g}^{2}}{\partial \rho_{m}}\right)-\frac{1}{\left(1+L^{2} B_{g}^{2}\right)}\left(B_{g}^{2} \frac{\partial L^{2}}{\partial \rho_{m}}+L^{2} \frac{\partial B_{g}^{2}}{\partial \rho_{m}}\right)$
Geometrical buckling depends solely on the geometry at first order:

$$
\alpha_{F}=\left.\frac{1}{F} \frac{\partial F}{\partial \rho_{m}}\right|_{T_{m}} \approx-\frac{B_{g}^{2}}{\left(1+\tau_{t h} B_{g}^{2}\right)} \frac{\partial \tau}{\partial \rho_{m}}-\frac{B_{g}^{2}}{\left(1+L^{2} B_{g}^{2}\right)} \frac{\partial L^{2}}{\partial \rho_{m}}
$$

For a large reactor, it is assumed that a decrease in density causes an increase in leakage of epithermal and thermal neutrons that is inversely proportional to the moderator density for first approximation. Hence, the coefficient $\alpha_{F}$ is positive and its contribution to the MTC is negative. The control/capture means for the reactor may be modeled in a very simplified way by decomposing the effect of rods as a function of the number of inserted rod steps $n$ and their reactive worths $w\left(n, T_{b}\right)$.

The rod worths increase as the rod temperature rises (owing to the Doppler effect with an increase of thermal captures).

$$
C_{r o d s}=1-n w\left(n, T_{b}\right)
$$

In practice, the rod temperature is close to that of the moderator, hence:
$\alpha_{T_{m}}^{\text {rods }}=\left.\frac{1}{C_{\text {rods }}} \frac{\partial C_{\text {rods }}}{\partial T_{m}}\right|_{\rho_{m}}=-\frac{n}{C} \frac{\partial w}{\partial T_{m}}<0$ and $\alpha_{\rho_{m}}^{\text {rods }}=\left.\frac{1}{C_{\text {rods }}} \frac{\partial C_{\text {rods }}}{\partial \rho_{m}}\right|_{T_{m}}=-\frac{n}{C} \frac{\partial w}{\partial T_{m}} \frac{d T_{m}}{d \rho_{m}}>0$
For the soluble boron effect, a first approximation may be made using the following hypothesis:

$$
C_{\text {boron }}=\frac{\sum_{a}^{m}}{\sum_{a}^{m}+\sum_{a}^{\text {boron }}}=\frac{N_{m} \sigma_{a}\left(T_{m}\right)}{N_{m} \sigma_{a}\left(T_{m}\right)+N_{\text {boron }} \sigma_{a}^{\text {boron }}\left(T_{m}\right)}
$$

In this equation, changes in concentration prevail over changes in cross sections (moreover, the boron cross section is unaffected by the Doppler effect):

$$
\begin{aligned}
\alpha_{T_{m}}^{\text {boron }} & =\frac{1}{C_{\text {boron }}} \frac{\partial C_{\text {boron }}}{\partial T_{m}}=\left.\frac{1}{C_{\text {boron }}} \frac{\partial C_{\text {boron }}}{\partial \rho_{m}}\right|_{T_{m}} \frac{d \rho_{m}}{d T_{m}}+\left.\frac{1}{C_{\text {boron }}} \frac{\partial C_{\text {boron }}}{\partial T_{m}}\right|_{\rho_{m}} \\
& \approx-\left.C s t C_{B} \frac{\partial N_{m}}{\partial \rho_{m}}\right|_{T_{m}} \frac{d \rho}{d T_{m}}>0
\end{aligned}
$$

This is true so long as the amounts of boron atoms and of water molecules depend linearly on the specific boron concentration $C_{B}$ (not to be confused with the capture ratio $C_{\text {boron }}$ ). The spectral term, disregarded hitherto, is positive if a rise in water temperature leads to hardening of the spectrum, thereby decreasing boron capture, thus increasing the capture ratio $C_{\text {boron }}$ :

$$
\left.\frac{1}{C_{\text {boron }}} \frac{\partial C_{\text {boron }}}{\partial T_{m}}\right|_{\rho_{m}}>0
$$

It may be concluded that if the $M T C$ is negative in $P W R$, the contribution of the control rods is negative, contrary to boron contribution. Both are proportional to their anti-reactivity. At the end of the cycle, boron contribution fades out.

### 16.2.3 Pressure Effect

Given that water density is increased by rises in isothermal pressure but decreased by rises in isobaric temperature, it may be inferred that the two effects are of different signs. This effect is negligible for a $P W R$ close to its operating state point.

### 16.2.4 Graphite Moderator

If the moderator is in solid state (e.g. French $U N G G$ or the British Magnox), the moderator temperature effect depends on graphite expansion (Kahan and Gauzit 1957). The migration area varies with the moderator density as:
where:

$$
M^{2}=M_{r e f}^{2}\left(\frac{\rho_{m, r e f}}{\rho_{m}}\right)^{2}
$$

$$
\frac{\partial M^{2}}{\partial T}=-2 M_{r e f}^{2} \frac{\rho_{m, r e f}^{2}}{\rho_{m}^{3}} \frac{\partial \rho}{\partial T}=-2 \frac{M^{2}}{\rho_{m}} \frac{\partial \rho_{m}}{\partial T}
$$

For a large reactor: $k_{\text {eff }}=k_{\infty} /\left(1+M^{2} B^{2}\right)$. Subsequently, close to criticality, the approximation $k_{\infty} \approx 1+M^{2} B^{2}$ is warranted and by logarithmic derivation, we obtain:

$$
\frac{\partial k_{e f f}}{k_{e f f}}=\frac{\partial k_{\infty}}{k_{\infty}}-\frac{\partial M^{2} B^{2}}{1+M^{2} B^{2}} \approx \frac{\partial \varepsilon}{\varepsilon}+\frac{\partial \eta}{\eta}+\frac{\partial f}{f}+\frac{\partial p}{p}-\frac{\partial M^{2} B^{2}}{k_{\infty}}
$$

where:

$$
\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T} \approx-\frac{B^{2}}{k_{\infty}} \frac{\partial M^{2}}{\partial T}=2 \frac{B^{2} M^{2}}{k_{\infty} \rho_{m}} \frac{\partial \rho_{m}}{\partial T}
$$

The linear expansion coefficient $\alpha$ appears in the density change:

$$
\rho_{m}=\frac{\rho_{m, r e f}}{1+\alpha\left(T-T_{r e f}\right)^{3}}
$$

Finally, deriving this density law with respect to temperature we obtain:

$$
\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T} \approx-6 \alpha \frac{B^{2} M^{2}}{k_{\infty}} \approx-6 \alpha \frac{k_{\infty}-1}{k_{\infty}}<0
$$

To this effect, which always has a negative sign, the expansion of the core lattice must be added. Thus, the geometrical buckling $B^{2}$ is modified. By definition of the $k_{e f f}$ :

$$
\frac{\partial k_{e f f}}{k_{e f f}}=-2 M^{2} B \frac{k_{\infty}}{k_{e f f}\left(1+M^{2} B^{2}\right)^{2}} \partial B=-2 M^{2} B \frac{1}{\left(1+M^{2} B^{2}\right)} \partial B \approx-2 \frac{M^{2} B}{k_{\infty}} \partial B
$$

Hence:

$$
\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T} \approx-2 \frac{M^{2} B}{k_{\infty}} \frac{\partial B}{\partial T}
$$

For simplification purposes, the reactor is assumed to be spherical with expanding radius $R=R_{r e f}\left(1+\alpha\left(T-T_{r e f}\right)\right)$ and with geometrical buckling $B=\pi / R$. It can be deduced that:

$$
\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T} \approx 2 \frac{M^{2} B}{k_{\infty}} \frac{\pi}{R^{2}} \frac{\partial R}{\partial T}=2 \alpha \frac{M^{2} B^{2}}{k_{\infty}}=2 \alpha \frac{k_{\infty}-1}{k_{\infty}}
$$

A cylindrical core must be expanded both radially and axially and its buckling is given as $B^{2}=(\pi / H)^{2}+\left(j_{0,1} / R\right)^{2}$, which complicates the formulae. Nevertheless, the general conclusion remains the same. The expansion effect of the size of the graphite pile is positive but is still three times less than the negative effect of the graphite. Overall, the effect is weak, of the order of a few dozen pcm per degree of graphite temperature, and is thus far smaller than the effect of a liquid moderator.

For the resonance escape probability, (Poulter 1963, p. 641) proposed the law:

$$
p_{(\mathrm{T})}=p_{\left(20^{\circ} \mathrm{C}\right)}\left(1-17,010^{-5} \frac{1-p_{\left(20^{\circ} \mathrm{C}\right)}}{p_{\left(20^{\circ} \mathrm{C}\right)}}\left(T_{S[K]}-293_{[\mathrm{K}]}\right)\right)
$$

where $T_{S[\mathrm{~K}]}$ is the average fuel surface temperature. Appendix 2 of (Poulter, 1963) shows the semi-empirical correlations and adjustments used in the design of British Magnox reactors.

### 16.2.5 Neutron Spectrum Shift

When the moderator temperature rises, as seen in Chap. 7, the neutron spectrum shifts towards higher energies and "hardens". This effect impacts the cross sections of all the isotopes in the reactor and not only those in the moderator (Fig. 16.5).

Fig. 16.5 Hardening of thermal spectrum with moderator temperature


### 16.2.6 Void Effect

The voiding of a reactor must be considered during an accident. The moderator flows out through a breach located on the primary loop. By design, the void effect is negative for French $P W R$ with the usual fuel types. However, it may become hazardous beyond a given plutonium content (as in the case of MOX where the plutonium content exceeds $12 \%$ ). The absence of water, resulting in a decrease in the thermalizing power of the reactor, shifts the spectrum to higher energies where some even-even isotopes of plutonium or ${ }^{238} U$ may undergo fission. This increases the reactivity and the reactor becomes somewhat like a "fast-neutron" reactor. The total void effect for an infinite cell lattice of the three fuel types described previously shows that an increase in MOX content significantly decreases the safety margin to criticality. It should be noted that these calculations do not take into account the dropping of control rods, which accounts for the disadvantageous factor $f$ in the four-factor formula (Fig. 16.6).

In water-cooled piles, the foregoing effect is stabilizing for $P W R$ with fuel having a low plutonium content. However, for piles moderated by heavy water and cooled by light water, the decrease in absorption of light water (with a capture rate far higher than heavy water) may lead to stability problems.

For sodium-cooled fast reactors, ${ }^{4}$ the sodium void effect has several consequences (Hummel and Okrent 1970, p. 82). First, it promotes neutron leakage from the fissile zone, which is beneficial for safety. However, the decreased capture on sodium and, above all, the spectrum shift to a pure fission spectrum results in a positive void coefficient, especially for plutonium fuel (for uranium fuel, the

Reactivity effect of complete voiding


Fig. 16.6 Reactivity effect of complete voiding (moderating ratio $=1.66$ )

[^334]effect is almost zero). Using certain design tricks such as reducing the size of the pile, using thinner solutions, or facilitating the voiding of the upper plenum, the void coefficient may be decreased or rendered negative. Unfortunately, limiting the core size or the breeding gain is not compatible with the design of an industrial reactor. The sodium void effect may be partial if a rise in the sodium temperature causes it to boil, leading to a void fraction.

### 16.3 Boron Effect in Pressurized Water Reactors

### 16.3.1 Differential Efficiency of Boron

The boron effect is not a temperature effect, yet it is often associated with neutronic reactivity feedback. Reactivity control throughout the cycle is achieved by gradually decreasing the amount of boric acid diluted in the primary-loop water. Starting from an initial concentration of $1000-1500 \mathrm{ppm}$ at BOC, it is diluted up to the natural cycle length, the burn-up at which the reactor is just critical without any boron. The boron differential effect is around $-8 \mathrm{pcm} / \mathrm{ppm}$ in a $U O X$ reactor. This value is very sensitive to the spectrum and falls to $-2 \mathrm{pcm} / \mathrm{ppm}$ in a $M O X$ spectrum.

This decrease in integral boron efficiency for $M O X$ reactors requires increase of the boron concentration at start-up or the use of other means of reactivity control (rods, burnable neutron poison such as gadolinium, in the fuel) since the boron concentration cannot be increased indefinitely (see paragraph below). Besides, even if it were possible, the risk of boron crystallization in water by saturation at a given temperature is not negligible. Nonetheless, a positive MTC would be reached well before boron saturation in water. Besides, the amount of boron is also limited in a safety context to prevent dilution accidents. The boron differential effect is always negative but varies significantly according to the loading pattern (Fig. 16.7).

## Boron differential effect



Fig. 16.7 Boron differential effect computed for a 500 ppm change in an under-moderated lattice (1.66)

### 16.3.2 Boron Effect on the Moderator Differential Coefficient

Another effect of the boron particularly important for the safety concerns the differential moderator differential coefficient. The more the boron concentration is important and the more this coefficient, usually negative, increases. Figure 16.8 shows that from 1500 ppm , this coefficient becomes positive at low temperature, and that from 2000 ppm , this one becomes positive below $180^{\circ} \mathrm{C}$. The negativity of this differential moderator coefficient during operation is a crucial element of safety in the case of a power excursion, because it allows a strong introduction of antireactivity as far as the temperature of the water increases. In operation, it is at the beginning of the cycle that the boron concentration is strongest. It is thus at this


Fig. 16.8 Boron effect on the moderator differential effect (UOX, 3.25\%, natural boron)
moment that it is necessary to watch over not to exceed a too strong boron concentration. The solution spends by the implementation of consumable poisons mixed in the solid fuel (gadolinium oxide for example) or of fixed (and further removed) absorbing rods placed in some tube guides (Pyrex glasses with boron carbide inclusion).

### 16.4 Power Coefficient

The fuel temperature is not easily obtained in a power reactor. Instead, the differential power coefficient is used:

$$
\alpha_{P} \equiv \frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial P}=\frac{1}{k_{e f f}} \frac{\partial k_{e f f}}{\partial T_{e f f}} \frac{\partial T_{\text {eff }}}{\partial P}
$$

where $T_{\text {eff }}$ is the mean effective temperature, a notion described in the chapter on the Doppler effect. This coefficient is around -2 to $-10 \mathrm{pcm} / \%$ Nominal power.

### 16.5 Feedback Modeling

(Silvennoinen 1976, p. 202)
The calculation of neutronic feedback involves computation of the thermal properties of materials within the core and of their impact on cross sections. It is assumed that the temperatures and densities at all points in the core are known, although this determination (thermalhydraulics) is outside the scope of this book. Very broadly, the change in macroscopic cross section may be written in terms of its partial derivatives with respect to certain feedback parameters. Let CRN (for Contre-Reactions Neutroniques in French) be the feedback parameter tuple previously described, i.e. ( $T_{\text {mod }}, \rho_{\text {mod }}, T_{\text {fuel }}, N_{X e}, N_{B}, N_{i}, \ldots$ ) where $N_{i}$ is the concentration of an additional isotope having a feedback effect (other than xenon135 and boron). Xenon-135, being the most absorbing fission product, is considered separately in all international models. It is supposed that the microscopic depletion of these isotopic feedback parameters is known in the fuel (or water for boron). It is further assumed that the cross section values for the reference feedback parameter tuple are known, i.e. $C R N^{0}=\left(T_{\text {mod }}^{0}, \rho_{\text {mod }}^{0}, T_{\text {comb }}^{0}, N_{X e}^{0}, N_{B}^{0}, N_{i}^{0}, \ldots\right)$. This parameter vector is chosen such that it corresponds to the standard state of the reactor: this is the "center" of the possible feedback parameter grid. Let $N$ be the number of isotopes required to ideally describe the macroscopic cross section and $n$ the number of isotopes considered as the independent feedback parameter (other than xenon-135 and boron-10). The cross section affected by feedback from a reference state 0 is modeled as follows using a Taylor series up to order 1 :

$$
\begin{aligned}
\Sigma_{a}^{C R N}= & \Sigma_{a}^{C R N^{0}}+\frac{\partial \Sigma_{a}}{\partial T_{\mathrm{mod}}} \Delta T_{\mathrm{mod}}+\frac{\partial \Sigma_{a}}{\partial \rho_{\mathrm{mod}}} \Delta \rho_{\mathrm{mod}}+\frac{\partial \Sigma_{a}}{\partial T_{\text {fuel }}} \Delta T_{\text {fuel }}+\frac{\partial \Sigma_{a}}{\partial N_{X e}} \Delta N_{X e} \\
& +\frac{\partial \Sigma_{a}}{\partial N_{B}} \Delta N_{B}+\sum_{i=1}^{n} \frac{\partial \Sigma_{a}}{\partial N_{i}} \Delta N_{i}
\end{aligned}
$$

Where the effect of the feedback parameter is marked, the expansion can be extended to order 2, which includes mixed terms. Using $C R N_{i}$ for the $i$ th feedback parameter, the cross section may be expressed for $M$ feedback parameters as:

$$
\begin{aligned}
\Sigma_{a}^{C R N}= & \Sigma_{a}^{C R N^{0}}+\sum_{i=1}^{M} \frac{\partial \Sigma_{a}}{\partial C R N_{i}} \Delta C R N_{i}+\frac{1}{2} \sum_{i=1}^{M} \frac{\partial^{2} \Sigma_{a}}{\partial C R N_{i}^{2}}\left(\Delta C R N_{i}\right)^{2} \\
& +\sum_{i \neq j} \frac{\partial^{2} \Sigma_{a}}{\partial C R N_{i} \partial C R N_{j}} \Delta C R N_{i} \Delta C R N_{j}+\ldots
\end{aligned}
$$

Physical analysis of the weight for the differential feedback coefficients determines the order up to which a given parameter must be expanded in the formula. Given that the density of water may be expected to be an influential parameter for $P W R$, it is thus expanded at higher orders. If a macroscopic cross section (e.g. absorption) is developed using these $N$ physical elements, by definition:

$$
\Sigma_{a}^{C R N}=\sum_{i=1}^{N} N_{i} \sigma_{a}^{i}=\Sigma_{a}^{r e s}+N_{X e} \sigma_{X e}+N_{B} \sigma_{B}+\sum_{i=1}^{n} N_{i} \sigma_{a}^{i}
$$

The residual macroscopic cross section $\sum_{a}^{r e s}$ represents the absorption of the remaining isotopes which are not considered as feedback parameters. The partial derivative of $\Sigma_{a}$ with respect to any feedback parameter (e.g. moderator temperature) is expressed as:

$$
\begin{aligned}
\frac{\partial \Sigma_{a}}{\partial T_{\mathrm{mod}}} & =\frac{\partial\left(\Sigma_{a}^{r e s}+N_{X e} \sigma_{X e}+N_{B} \sigma_{B}+\sum_{i=1}^{n} N_{i} \sigma_{a}^{i}\right)}{\partial T_{\mathrm{mod}}} \\
& =\frac{\partial \Sigma_{a}^{r e s}}{\partial T_{\mathrm{mod}}}+N_{X e} \frac{\partial \sigma_{X e}}{\partial T_{\mathrm{mod}}}+N_{B} \frac{\partial \sigma_{B}}{\partial T_{\mathrm{mod}}}+\sum_{i=1}^{n} N_{i} \frac{\partial \sigma_{a}^{i}}{\partial T_{\mathrm{mod}}}
\end{aligned}
$$

and similarly for moderator density and fuel temperature. For xenon (in fact xenon-135), the following is used:

$$
\frac{\partial\left(N_{X e} \sigma_{X e}\right)}{\partial N_{X e}}=\left(\sigma_{X e}+N_{X e} \frac{\partial \sigma_{X e}}{\partial N_{X e}}\right)
$$

Hence: $\frac{\partial \Sigma_{a}}{\partial N_{X e}}=\frac{\partial \Sigma_{a}^{r e s}}{\partial N_{X e}}+\left(\sigma_{X e}+N_{X e} \frac{\partial \sigma_{X e}}{\partial N_{X e}}\right)+N_{B} \frac{\partial \sigma_{B}}{\partial N_{X e}}+\sum_{i=1}^{n} N_{i} \frac{\partial \sigma_{a}^{i}}{\partial N_{X e}}$

Boron is considered in the same way as xenon. For all other feedback parameter isotopes, j (thus modeled with microscopic depletion in the core calculation codes), the following is obtained:

$$
\frac{\partial \Sigma_{a}}{\partial N_{j}}=\frac{\partial \Sigma_{a}^{r e s}}{\partial N_{j}}+N_{X e} \frac{\partial \sigma_{X e}}{\partial N_{j}}+N_{B} \frac{\partial \sigma_{B}}{\partial N_{j}}+\left(\sigma_{j}+N_{j} \frac{\partial \sigma_{j}}{\partial N_{j}}\right)+\sum_{i=1, i \neq j}^{n} N_{i} \frac{\partial \sigma_{a}^{i}}{\partial N_{j}}
$$

The partial derivatives of microscopic cross sections with respect to the amount of other isotopes should be pointed out as they represent their respective spectral effect. Thus an absorbing isotope modifies the spectrum, thereby leading to modification of the cross sections of the other isotopes. This effect is referred to in the literature as historical correction to emphasize the fact that it is produced by drift in the fuel history during microscopic depletion, carried out at feedback conditions other from the reference conditions. These may be large enough (of the order of $10 \%$ of a macroscopic cross section) to cause significant errors during the cycle if overlooked. The goal of a generalized feedback model is to choose the predominant terms among the partial derivatives of macroscopic cross sections and to evaluate these derivatives in an analytical or tabulated manner with sufficient precision for industrial use (time/simplicity/precision ratio). A particular use of the feedback model is for a cross section in a medium, with almost unvarying physical properties except for its concentration. This is the case for fast reactors, where cross sections do not vary much because of the hard spectrum, even with burn-up. Besides, the fission products are less absorbing than in $P W R$. ${ }^{5,6}$ Hence:

$$
\Sigma(t)=\Sigma\left(t_{0}\right)+\left(t-t_{0}\right) \frac{d \Sigma}{d t}+\frac{\left(t-t_{0}\right)^{2}}{2} \frac{d^{2} \Sigma}{d t^{2}}+\ldots
$$

where $\frac{d \Sigma}{d t}=\frac{d\left(\sum_{i=1}^{N} N_{i} \sigma_{i}\right)}{d t}=\sum_{j=1}^{N} \frac{\partial\left(\sum_{i=1}^{N} N_{i} \sigma_{i}\right)}{\partial N_{j}} \frac{d N_{j}}{d t}=\sum_{j=1}^{N}\left(\sigma_{j}+N_{j} \frac{\partial \sigma_{j}}{\partial N_{j}}\right) \frac{d N_{j}}{d t}$
The proposed reasoning as a function of time may also be extended to burn-up in a similar way.

[^335]
### 16.5.1 A Simple Model: Power Feedback

One of the simplest models considered is to account for the power effect in two-group diffusion calculation for a $P W R$. A change in normalized power $P$ causes a change, assumed linear, of the water density:

$$
\Delta \rho_{\mathrm{H}_{2} \mathrm{O}}=(P-1) \frac{d \rho_{\mathrm{H}_{2} \mathrm{O}}}{d P}
$$

This density change induces two major effects: first, the variation of the absorption cross section $\Delta \Sigma_{a}$, transport one $\Delta \Sigma_{t}$ and scattering one $\Delta \Sigma_{s}$, with the same sign as $\Delta \rho_{\mathrm{H}_{2} \mathrm{O}}$ and linked to the change in the amount of water molecules $\mathrm{N}_{\mathrm{H}_{2} \mathrm{O}}$ :

$$
\Delta \Sigma=\operatorname{Voliq} N_{\mathrm{H}_{2}} O \sigma_{\mathrm{H}_{2}} O \frac{d \rho_{\mathrm{H}_{2} \mathrm{O}}}{\rho_{\mathrm{H}_{2} \mathrm{O}}}
$$

where Voliq is the proportion of water in the material.
The change in total cross section induces a change of the diffusion coefficient:

$$
\Delta D=D \frac{\Delta \Sigma_{t}}{\Sigma_{t}+\Delta \Sigma_{t}}
$$

In addition, the hardening of the spectrum due to a simultaneous change in the slowing-down capacity of water (a change in slowing-down density) mainly impacts the fast absorption cross section, which is usually expressed as a logarithmic derivative:

$$
\frac{d \Sigma}{\Sigma}=s_{[-]} \frac{d \rho_{\mathrm{H}_{2} \mathrm{O}}}{\rho_{\mathrm{H}_{2} \mathrm{O}}}
$$

The power rise leads to an increase in fuel temperature which induces a Doppler effect. The latter mainly affects the absorption cross section with an experimental saturation effect modeled empirically by:

$$
\Delta \Sigma_{a, 1}=\frac{\alpha_{1} P}{1+\alpha_{2} P}-\frac{\alpha_{1}}{1+\alpha_{2}}
$$

The effect of the absorbing materials such as boron (of concentration $N_{B}$ ) and xenon (of concentration $N_{X e}$ ) on the absorption cross sections (hence, the total cross section also) is considered linear:

$$
\Delta \Sigma_{a}=\Delta N_{B} \sigma_{B}+\Delta N_{X e} \sigma_{X e}
$$

The transfer cross section $\Sigma_{1 \rightarrow 2}$ varies according to the law:

$$
\frac{\Sigma_{1 \rightarrow 2}}{\Sigma_{a, 1}+\Sigma_{1 \rightarrow 2}}=e^{-\frac{\Sigma_{a, 1}}{\Sigma_{s}}}
$$

The coefficients used in the previous equations are calculated once only by the different branch calculations (for each feedback tuple) using a transport code before the core code. This simple and fast model is implemented in the JASON ${ }^{7}$ pin-by-pin diffusion code at $E D F$. This methodology allows calculation of the critical boron concentration with a dispersion of less than 30 ppm .

### 16.5.2 An Advanced Feedback Model: The Lefebvre-Seban Model



Jean-Claude Lefebvre (1939-2011) (on the left) spent his whole career until 1999 at EDF after obtaining Master's in Reactor Physics in 1967. He helped lay the foundations of the official computation scheme for EDF PWR cores by programming the JONAS pin-cell diffusion code and the JANUS 2D core code. His theoreticals, though disarmingly simple, were sufficiently precise to stand the test of time for the past 30 years. As a result, the computation scheme to which he contributed significantly, so much so that he may be considered as its "founding father", is still in use. and will indeed be used to compute the future $E P R$ reactor. His major theoretical contributions are the two-group neutron feedback model for $E D F$, together with Roger Seban, and the official reflector model alongside Philippe Lebigot. (Courtesy Lefebvre/Courtesy Seban)

[^336]

Roger Seban (1949-) (on the right) obtained his "Génie Atomique" engineering degree (1974), after a Master's in Reactor Physics. His work as a freshly-qualified engineer in October 1976 at SEPTEN with Jean-Claude Lefebvre led to the design of an industrial feedback model to challenge the Framatome computation chain, obtained via its license with Westinghouse and which EDF does not hold. This pragmatic and fast model runs a large number of daily loading calculations with the pre-calculations obtained from the CEA transport code APOLLO-1. Roger Seban was appointed head of the Nuclear Mechanical Department at $E D F / C N E N$ before working as technical director of $E D F / C N E P E$ from 2001 to 2004. He then held a number of high-responsibility posts in China on reactor projects at Daya Bay and Ling'Ao. He returned to the $R \& D$ division of $E D F$ in 2013 as head of the "Future Reactor" project.

In the early 1980s, J. C. Lefebvre and R. Seban proposed a new model for the main feedback effects. ${ }^{8}$ This model was simple and efficient for a two-group diffusion calculation with a cut-off energy at $E_{c}=0.625 \mathrm{eV}$, corresponding to a cut-off temperature $T_{c}=7243 \mathrm{~K}$ such that $k T_{c}=0.625 \mathrm{eV}$ and at a lethargy $u_{c}$. Disregarding absorption when compared to the slowing-down outside a narrow resonance ( $\gamma \Sigma_{a} \ll \xi \Sigma_{s}$ ), we saw in the chapter on slowing down that the slowingdown density is given by the Greuling-Goertzel model:

$$
\text { Slowing-down density : } \begin{cases}q(u)=e^{-\frac{\sum_{a}}{\xi \sum_{s}} u} & \text { if } 0<u<u_{\text {res }},  \tag{16.1}\\ q(u)=e^{-\frac{\Sigma_{a}}{\xi \sum_{s}} u} e^{-\frac{\Gamma}{\xi}} & \text { if } u_{\text {res }}<u<u_{c},\end{cases}
$$

[^337]The term $p_{\text {res }} \approx e^{-\frac{\Gamma}{\xi}}$ is the probability of escaping a narrow resonance $(\Gamma \ll \xi)$. The flux expression in the fast group (lethargy lower than the cut-off) is as follows:

$$
\begin{aligned}
\Phi_{1} & =\int_{0}^{u_{c}} \Phi(u) d u=\int_{0}^{u_{c}} \frac{q(u)}{\xi \Sigma_{s}(u)+\gamma \Sigma_{a}(u)} d u \\
& =\int_{0}^{u_{R}} \frac{e^{-\frac{\Sigma_{a}}{\xi \Sigma_{s}} u}}{\xi \Sigma_{s}(u)+\gamma \Sigma_{a}(u)} d u+\int_{u_{R}}^{u_{c}} \frac{e^{-\frac{\Sigma_{a}}{\xi \Sigma_{s}} u e^{-\frac{\Gamma}{\xi}}} \frac{\xi \Sigma_{s}(u)+\gamma \Sigma_{a}(u)}{l} d u}{} .
\end{aligned}
$$

Thus:

$$
\Phi_{1} \approx \frac{1}{\Sigma_{a}}\left[1-e^{-\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u_{r e s}}+e^{\left.\left.\left.-\frac{\Gamma}{\xi \cdot} \cdot\left(e^{-\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u_{r e s}}-e^{-\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u_{c}}\right)\right] .\right] ~\right] . ~}\right.
$$

Using a first order Taylor expansion of the exponentials:

$$
e^{-\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u_{r e s}} \approx 1-\frac{\Sigma_{a}}{\xi \Sigma_{s}+\gamma \Sigma_{a}} u_{r e s}
$$

The equation for the fast flux is:
Fast flux in the Lefebvre-Seban model :

$$
\begin{equation*}
\Phi_{1}=\frac{1}{\xi \Sigma_{s}+\gamma \Sigma_{a}}\left[u_{\text {res }}+\left(u_{c}-u_{\text {res }}\right) e^{-\frac{\Gamma}{\xi}}\right] \tag{16.2}
\end{equation*}
$$

The slowing-down current $q$ and the flux $\Phi_{1}$ change in particular with the boron concentration via the fast absorption cross section $\Sigma_{a}$, with the fuel temperature $T_{\text {fuel }}$ via the resonance width $\Gamma$ (the Doppler effect itself varies as $\sqrt{T_{\text {fuel }}}$ ), and with the water density $N_{\mathrm{H}_{2} \mathrm{O}}$ via the moderating power $\xi \Sigma_{s}$ and the fast absorption cross section $\Sigma_{a}$. The effect of other isotopes on the spectrum, and thus on the cross sections, is disregarded for the time-being. Introducing the absorption term into the thermalization equation twists the spectrum with respect to Maxwell's spectrum. J. Horowitz and O. Tretiakoff proposed that this twist be characterized as a discrepancy between the true spectrum and Maxwell's spectrum. In Chap. 7, we saw that this leads to the definition of the neutron density as:

$$
n(x)=m(x)+2 r_{H T} e(x)
$$

where $e(x)$ represents the coupling density between the fast and thermal domains and $r_{H T}$ is the spectral index related to the proportion of neutrons crossing the
cut-off energy. The spectral index $r_{H T}$ (characterizing coupling between the two domains) is written as:

$$
r_{H T}=\frac{q(x)}{v_{T} \xi \Sigma_{s}(x)}
$$

In a two-group model, the Horowitz-Tretiakoff spectral index is given as:

$$
\begin{equation*}
\text { Horowitz-Tretiakoff spectral index : } r_{H T}=\frac{\sqrt{\frac{T_{0}}{T}}}{\frac{\xi \Sigma_{s}}{\hat{\Sigma}_{a}}+2 \sqrt{\frac{T_{0}}{T_{c}}}} \tag{16.3}
\end{equation*}
$$

From the expression of $r_{H T}$, it may be deduced that the operating parameter effects can be applied to the effective cross sections (the moderating power $\xi \Sigma_{s}$ is almost constant). However, in diffusion codes, energy (usually two groups)averaged cross sections are employed. The use of effective cross sections requires a relation linking them to energy-averaged cross sections. For this purpose, a function $\Phi_{\text {condensed }}$ is needed to characterize the number of neutrons at each point, as well as the reaction rate distribution. Therefore, the following is defined:

$$
\Sigma_{\text {condensed }} \Phi_{\text {condensed }}=\int_{0}^{\infty} \Sigma(v) \Phi(v) d v .
$$

Thus, $\Phi_{\text {condenseed }}$ needs only to be defined to deduce a definition for $\Sigma_{\text {condense }}$. $\Phi_{\text {condense }}$ is normally assumed to be the integral of the flux spectrum:

$$
\Phi_{\text {condensed }}=\bar{\Phi}=\int_{0}^{\infty} v n(v) d v
$$

The average cross section is thus:

$$
\Sigma_{\text {condensed }}=\bar{\Sigma}=\frac{\int_{0}^{\infty} \Sigma(v) v n(v) d v}{\int_{0}^{\infty} v n(v) d v}
$$

Another condensation method consists in using the Westcott effective cross sections defined as:

$$
\hat{\Sigma}=\frac{\int_{0}^{\infty} \Sigma(v) v n(v) d v}{v_{0} \int_{0}^{\infty} n(v) d v}
$$

In the $C E A$ codes APOLLO1 and APOLLO2, the relation between effective and average cross sections is obtained through a parameter called Unita defined as:

$$
\frac{\hat{\Sigma}_{a}}{\bar{\Sigma}_{a}}=\frac{\int_{0}^{v_{c}} \varphi(v) d v}{v_{0} \int_{0}^{v_{c}} n(v) d v}=\frac{\int_{0}^{v_{c}} v n(v) d v}{v_{0} \int_{0}^{v_{c}} n(v) d v}=\frac{\bar{v}}{v_{0}}=\frac{1}{\text { Unita }}
$$

This parameter is determined once the neutron density representation $n(x)$ is known. Indeed:

$$
\text { Unita }=\frac{v_{0} \int_{0}^{x_{c}}[m(x)+2 r e(x)] d x}{\int_{0}^{x_{c}} v[m(x)+2 r e(x)] d x}=\frac{1+2 r \bar{e}}{\bar{x}_{m}+2 r \bar{x}_{e}} \frac{v_{0}}{v_{T}}
$$

where: $\bar{e}=-\sqrt{\frac{T}{T_{c}}}, \bar{x}_{m}=\frac{2}{\sqrt{\pi}}, \bar{x}_{e}=\bar{x}_{e}^{\text {ref }}-\log \sqrt{\frac{T}{T^{r e f}}}$ where $T$ is the moderator temperature, $T_{c}$ the cut-off temperature and $T^{r e f}$ the reference cut-off temperature.

The evaluation of the spectral index leads to the determination of the Unita parameter to compute the average cross sections used in the diffusion codes. In the Lefebvre-Seban model, the nuclear parameters (cross sections, neutron flux, slowing-down density) are tabulated as a function of burn-up and are correlated with operating parameters (fuel temperature, moderator temperature, moderator density, boron concentration, xenon concentration). In the fast energy domain, the slowing-down density and the fission cross section are influenced by changes in the boron concentration, fuel temperature (Doppler effect) and water density. Moreover, the scattering and transfer cross sections are also affected by changes in the moderator density. In the thermal energy domain, the neutron flux, the fission cross section and the transfer cross section are influenced by the moderator temperature and, the boron and xenon concentrations. Finally, the ratio of the production cross section to the amount of absorption is modified by changes in the moderator density. Doppler feedback is modeled with three coefficients: $\alpha_{q D}, \alpha_{\Phi D}$ and $\alpha_{f D}$ :

Doppler feedback : $\left\{\begin{array}{c}\ln \left(\frac{1}{q}\right)-\ln \left(\frac{1}{q^{r e f}}\right)=\alpha_{q D}\left(\sqrt{T_{\text {fuel }}}-\sqrt{T_{\text {fuel }}^{\text {ref }}}\right) \\ \Phi_{1}-\Phi_{1}^{\text {ref }}=\alpha_{\Phi D}\left(\sqrt{T_{\text {fuel }}}-\sqrt{T_{\text {fuel }}^{\text {ref }}}\right) v \Sigma_{f_{1}}-v \Sigma_{f_{1}}^{\text {ref }}=\alpha_{f D}\left(\sqrt{T_{\text {fuel }}}-\sqrt{T_{\text {fuel }}^{\text {ref }}}\right)\end{array}\right.$

The boron effect, with $N_{B}$ the concentration of boron nuclei per $\mathrm{cm}^{3}$, is modeled using three coefficients, $\alpha_{q B}, \alpha_{\Phi B}$ and $\alpha_{f B}$ :

Boron feedback : $\left\{\begin{array}{c}\ln \left(\frac{1}{q}\right)-\ln \left(\frac{1}{q^{r e f}}\right)=\alpha_{q B}\left(N_{B}-N_{B}^{r e f}\right) \frac{N_{W}^{r e f}}{N_{W}} \\ \Phi_{1}-\Phi_{1}^{r e f}=\alpha_{\Phi B}\left(N_{B}-N_{B}^{r e f}\right)\end{array} \quad v \Sigma_{f_{1}}-v \Sigma_{f_{1}}^{r e f}=\alpha_{f B}\left(N_{B}-N_{B}^{r e f}\right)\right.$

The water density effect is modeled using five coefficients:

Water density effect : $\left\{\begin{array}{r}\ln \left(\frac{1}{q}\right)-\ln \left(\frac{1}{q^{r e f}}\right)=\alpha_{q W}\left[\frac{N_{W}-N_{W}^{r e f}}{N_{W} N_{W}^{r e f}}\right] \\ \Phi_{1}-\Phi_{1}^{r e f}=\alpha_{\Phi W}\left[\frac{N_{W}-N_{W}^{r e f}}{N_{W} N_{W}^{r e f}}\right] \quad v \Sigma_{f_{1}}-v \Sigma_{f_{1}}^{r e f}=\alpha_{f W}\left(q-q^{r e f}\right) \\ \Sigma_{t r_{1}}-\Sigma_{t r_{1}}^{r e f}=\alpha_{t W}\left(N_{W}-N_{W}^{r e f}\right) \quad \\ \frac{\left(\xi \Sigma_{s}-\xi \Sigma_{s}^{r e f}\right)}{\xi \Sigma_{s}^{r e f}}=\alpha_{\xi W}\left[\frac{N_{W}-N_{W}^{r e f}}{N_{W}^{r e f}}\right]\end{array}\right.$
$N_{W}$ represents the amount of moderator molecules per $\mathrm{cm}^{3}$ and $\Sigma_{t r_{1}}$ is the fast transport cross section. The feedbacks also modify the thermal cross sections. The moderator density effect is difficult to model to obtain a satisfactory expression for the changes in the fission and absorption effective cross sections. Hence, the effective absorption and the fuel multiplication coefficient $\eta=v \Sigma_{f} / \Sigma_{a_{2}}$ are modeled as:

Thermal effect of water density :

$$
\left\{\begin{array}{c}
\Sigma_{t r_{2}}-\Sigma_{t r_{2}}^{r e f}=\beta_{t W}\left(N_{W}-N_{W}^{r e f}\right)  \tag{16.7}\\
\frac{\hat{\Sigma}_{a_{2}}-\hat{\Sigma}_{a_{2}}^{r e f}}{\hat{\Sigma}_{a_{2}}^{r e f}}=\beta_{a W}\left(\frac{N_{W}-N_{W}^{r e f}}{N_{W}^{r e f}}\right) \quad \frac{\eta-\eta^{r e f}}{\eta^{r e f}}=\beta_{\eta W}\left(\frac{N_{W}-N_{W}^{r e f}}{N_{W}^{r e f}}\right)
\end{array}\right.
$$

To simplify the equations, let:

$$
x \equiv \frac{N_{W}-N_{W}^{r e f}}{N_{W} N_{W}^{r e f}} \text { and } X \equiv \frac{N_{W}-N_{W}^{r e f}}{N_{W}^{r e f}}
$$

Then:

$$
\left\{\begin{array}{l}
\ln \left(\frac{1}{q}\right)-\ln \left(\frac{1}{q^{r e f}}\right)=\alpha_{q W} x \\
\Phi_{1}-\Phi_{1}^{r e f}=\alpha_{\Phi W} x \\
\frac{\eta-\eta^{r e f}}{\eta^{r e f}}=\beta_{\eta W} X
\end{array}\right.
$$

Studies have evaluated the precision of this model depending on the calculation of the coefficients $\alpha_{q W}, \alpha_{\Phi W}$ and $\beta_{\eta W}$. A simple method to determine these coefficients is by use of the difference between two calculations carried out at two different water densities. Thus, two values of $x$ are obtained, for example one at nominal density $0.7169 \mathrm{~g} / \mathrm{cm}^{3}$ and the other at a hotter density (left derivative of the nominal operation point) of $0.5 \mathrm{~g} / \mathrm{cm}^{3}$. A colder density of $0.8 \mathrm{~g} / \mathrm{cm}^{3}$ may be chosen for the right derivative. The plots in $x$ (or in $X$ for the fuel multiplication coefficient $\eta$ ) obtained by this approach may be compared to those for precise calculations carried out with the APOLLO2 code for each density (called 'GAB' calculations).

The results (Figs. 16.8, 16.9, 16.10 and 16.11) show that there is a good agreement for the calculations on the right and on the left, especially for hotter conditions than the nominal ones $(x<0)$. The calculations with the right derivative as 0.8 improves the results for the following parameters: $\ln (1 / q), \eta$ and $\Phi_{1}$ for densities lower than $0.7169 \mathrm{~g} / \mathrm{cm}^{3}$, which may seem paradoxical.

Further studies have shown that this model is not valid at very low densities $\left(<0.3 \mathrm{~g} / \mathrm{cm}^{3}\right)$ for severe accidents in which linear behavior in $\Delta N_{W}$ is no longer an acceptable approximation, as is the dissociation of feedback effects. The model may be upgraded using polynomials of degree two or three, and introducing mixed effects for the water density on other feedbacks. Water temperature affects cross sections through the Doppler effect:

Thermal effect of water temperature :

$$
\left\{\begin{array}{l}
\frac{\hat{\Sigma}_{a_{2}}-\hat{\Sigma}_{a_{2}}^{r e f}}{\hat{\Sigma}_{a_{2}}^{r e f}}=\beta_{a T}\left(\frac{\sqrt{T_{\mathrm{H}_{2} \mathrm{O}}}-\sqrt{T_{\mathrm{H}_{2} \mathrm{O}}^{\text {ref }}}}{\sqrt{T_{\mathrm{H}_{2} \mathrm{O}}^{\text {ref }}}}\right)  \tag{16.8}\\
\frac{v \hat{\Sigma}_{f_{2}}-v \hat{\Sigma}_{f_{2}}^{r e f}}{v \hat{\Sigma}_{f_{2}}^{r e f}}=\beta_{f T}\left(\frac{\sqrt{T_{\mathrm{H}_{2} \mathrm{O}}}-\sqrt{T_{\mathrm{H}_{2} \mathrm{O}}^{\text {ref }}}}{\sqrt{T_{\mathrm{H}_{2} \mathrm{O}}^{\text {ref }}}}\right)
\end{array}\right.
$$



Fig. 16.9 Precision of the Lefebvre-Seban model on the fuel multiplication coefficient for $8.65 \%$ MOX (Parity MOX project). The most precise values are those of the "GAB" points. The linear model is obtained by the left derivative $\left(0.05 \mathrm{~g} / \mathrm{cm}^{3}\right)$ and on the right $\left(0.8 \mathrm{~g} / \mathrm{cm}^{3}\right)$, with respect to a reference density of $0.7169 \mathrm{~g} / \mathrm{cm}^{3}$. (EDF calculations performed by F. Hollinger/F. Adel in 2003)


Fig. 16.10 Precision of the Lefebvre-Seban model for fast flux (conditions as for Fig. 16.8)


Fig. 16.11 Precision of the Lefebvre-Seban model for the logarithm of the slowing-down density (conditions as for Fig. 16.8)

Boron concentration has a linear influence over transport, absorption and fission cross sections, as does xenon-135:

Boron and xenon thermal effects :

$$
\left\{\begin{array} { c } 
{ \Sigma _ { t r _ { 2 } } - \Sigma _ { t r _ { 2 } } ^ { r e f } = \beta _ { t B } ( N _ { B } - N _ { B } ^ { r e f } ) }  \tag{16.9}\\
{ \hat { \Sigma } _ { a _ { 2 } } - \hat { \Sigma } _ { a _ { 2 } } ^ { r e f } = \beta _ { a B } ( N _ { B } - N _ { B } ^ { r e f } ) } \\
{ v \hat { \Sigma } _ { f _ { 2 } } - v \hat { \Sigma } _ { f _ { 2 } } ^ { r e f } = \beta _ { f B } ( N _ { B } - N _ { B } ^ { r e f } ) }
\end{array} \left\{\begin{array}{c}
\Sigma_{t r_{2}}-\Sigma_{t r_{2}}^{r e f}=\beta_{t X e}\left(N_{X e}-N_{X e}^{r e f}\right) \\
\hat{\Sigma}_{a_{2}}-\hat{\Sigma}_{a_{2}}^{r e f}=\beta_{a X e}\left(N_{X e}-N_{X e}^{r e f}\right) \\
v \hat{\Sigma}_{f_{2}}-v \hat{\Sigma}_{f_{2}}^{r e f}=\beta_{f X e}\left(N_{X e}-N_{X e}^{r e f}\right)
\end{array}\right.\right.
$$

The average cross sections in the thermal group are determined using the effective cross sections and the Unita parameter. First, the $r_{H T}$ parameter is computed in nominal conditions (denoted ref):

$$
r_{H T}^{r e f}=\frac{\sqrt{\frac{T_{0}}{T_{H_{2} O}^{r e f}}}}{\frac{\xi \Sigma_{s}^{r e f}}{\hat{\Sigma}_{a_{2}}^{r e f}}+2 \sqrt{\frac{T_{0}}{T_{c}}}}
$$

In addition, the mean reduced speed weighted by the function $e(x)$ is also computed in the same conditions:

$$
\bar{x}_{e}^{r e f}=\int_{0}^{x_{c}} x e(x) d x=\frac{\left[1-2 r_{H T}^{r e f} \sqrt{\frac{T_{H_{2} O}^{r e f}}{T_{c}}}\right]}{2 r_{H T}^{r e f}(\text { Unita })^{r e f}} \sqrt{\frac{T_{0}}{T_{H_{2} O}^{r e f}}}-\frac{\bar{x}_{m}}{2 r_{H T}^{r e f}}
$$

Using the feedback models, new effective cross sections are obtained, along with the following new parameters:

$$
r_{H T}^{c r n}=\frac{\sqrt{\frac{T_{0}}{T_{H_{2} O}}}}{\frac{\xi \sum_{s}^{c r n}}{\hat{\Sigma}_{a_{2}}^{c r n}}+2 \sqrt{\frac{T_{0}}{T_{e}}}} \quad \quad \bar{x}_{e}^{c r n}=\bar{x}_{e}^{r e f}-\frac{1}{2} \ln \frac{T_{H_{2} O}}{T_{H_{2} O}^{r e f}}
$$

and, finally, the Unita parameter after applying feedback:

$$
(\text { Unita })^{c r n}=\frac{\left[1-2 r_{H T}^{c r n} \sqrt{\frac{T_{H_{2} O}}{T_{c}}}\right]}{\left(\bar{x}_{m}+2 r_{H T}^{c r} \bar{x}_{e}^{c r n}\right)} \sqrt{\frac{T_{0}}{T_{H_{2} O}}}
$$

The average cross sections in the thermal group are obtained using Unita:

$$
\left\{\begin{aligned}
& \hat{\Sigma}_{a_{2}}^{c r n}=\left(\text { Unita }^{c r n}\right. \\
& v \hat{\Sigma}_{f_{2}}^{r e ́ f} \\
& v \hat{\Sigma}_{f_{2}}^{c r n}=(\text { Unita })^{c r n} \\
& \hline \hat{\Sigma}_{f_{2}}^{r e f}
\end{aligned}\right.
$$

Without leakage, the slowing-down current $q$ and the integrated fast flux $\Phi_{1}$ are linked by the transfer cross section from group 1 to group $2 \Sigma_{r}: q\left(x_{c}\right)=\Sigma_{r} \Phi_{1}$. The infinite lattice hypothesis (zero buckling) relates the neutron quantities in the fast domain very simply. The neutron balance equations normalized to one produced neutron are:

$$
\left\{\begin{array}{c}
\Sigma_{a_{1}} \Phi_{1}+\Sigma_{r} \Phi_{1}=\frac{v \Sigma_{f_{1}} \Phi_{1}+v \Sigma_{f_{2}} \Phi_{2}}{k_{\text {eff }}}=1 \\
\Sigma_{a_{2}} \Phi_{2}-\Sigma_{r} \Phi_{1}=0
\end{array}\right.
$$

The cross sections $\Sigma_{a_{1}}$ and $\Sigma_{r}$ are deduced using the feedback on $\Phi_{1}$ and $q$. Nevertheless, the feedback model in the fast group is valid only in infinite lattice. Therefore, using "0" (zero-buckling calculation) and "crn" (calculation after applying neutron feedback):

$$
\Sigma_{r}^{0, c r n}=\frac{q^{0, c r n}}{\Phi_{1}^{0, c r n}} \quad \Sigma_{a_{1}}^{0, c r n}=\frac{1-q^{0, c r n}}{\Phi_{1}^{0, c r n}}
$$

However, in the APOLLO2 assembly calculations, the cross sections are usually homogenized using a non-zero critical buckling term, equal to the material buckling. Hence, in this model, leakage correction is necessary. The semi-empirical corrections used are :

Material buckling effect :

$$
\begin{align*}
& k_{\infty}^{0}=\frac{k_{\infty}}{1+B_{m}^{2}\left(a B_{m}^{2}+b\right)} \quad D_{1}^{0}=\frac{D_{1}}{1-\gamma B_{m}^{2}}, \gamma=3.942 \\
& v \Sigma_{f 1}^{0}=\frac{v \Sigma_{f 1}}{1-\beta B_{m}^{2}}, \beta=4.03 \quad \Sigma_{r}^{0}=\Sigma_{r} e^{\alpha} \frac{D_{1}}{\Sigma_{r}+\Sigma_{a 1}} B_{m}^{2}, \alpha=0.245 \tag{16.9}
\end{align*}
$$

The parameters $a$ and $b$ are determined from two APOLLO2 calculations for assemblies with two different enrichments. Neutron quantities without the " 0 " index are obtained from an APOLLO2 calculation with non-zero material buckling. The coefficients $\alpha, \beta$ and $\gamma$ come from an empirical fit. It should be pointed out that the thermal group values are not corrected for leakage. The fast cross sections including the leakage effect are determined by solving a second-order equation in $B_{m}^{2}$ iteratively:

$$
k_{e f f}=\frac{\Sigma_{r}^{c r n}}{\Sigma_{a_{1}}^{c r n}+\Sigma_{r}^{c r n}+D_{1}^{c r n} B_{m}^{2}}\left[\frac{v \Sigma_{f_{1}}^{c r n}}{\Sigma_{r}^{c r n}}+\frac{v \Sigma_{f_{2}}^{c r n}}{\Sigma_{a_{2}}^{c r n}+D_{2}^{c r n} B_{m}^{2}}\right]=1
$$

This resolution is carried out given that the cross sections also depend on the material buckling $B_{m}^{2}$ through the semi-empirical laws governed by Eq. 16.9. Since the cross sections have a physical sense in the latter, the roots are real. One is strongly negative, thus corresponding to a non-physical case in which the leakage is largely over-estimated with respect to the reaction rate in the medium. The other root may be positive or negative and is close to 0 -this is the value being sought. It has been observed that for densities lower than $0.3 \mathrm{~g} / \mathrm{cm}^{3}$, i.e. where there is a void
fraction above $60 \%$ at 70 bars, the homogeneous feedback model fails. For instance, beyond these conditions, the $k_{\infty}$ calculated with the model increases with the void fraction. This may be explained by the fact that there is a strong hypothesis in the calculation: the effect of the five parameters on the cross sections are taken to be uncoupled, and each effect is thus computed separately and added afterwards. However, although this hypothesis is valid in the standard operating range of the reactor, this is no longer the case when the density is decreased drastically. Indeed, feedback effects depend on the spectrum, which changes significantly when the moderator density varies. As for the fuel composition, the model accounts for the fact that the reference values of the parameters change during depletion to the reference feedback parameter values: $T_{H_{2} \mathrm{O}}^{r e f}=306^{\circ} \mathrm{C}$, $\rho_{\mathrm{H}_{2} \mathrm{O}}^{\text {ref }}=0.71 \mathrm{~g} / \mathrm{cm}^{3}, T_{\mathrm{UO}_{2}}^{\text {ref }}=600^{\circ} \mathrm{C}$-these are the average values in a reactor core. For this purpose, a linear correction with the historical moderator density is applied to the cross sections. This correction is defined locally in terms of burn-up by: ${ }^{9}$

$$
\rho_{\text {historical }}(\vec{r}, \tau)=\frac{\int_{0}^{\tau} \rho_{\mathrm{H}_{2} O}\left(\vec{r}, \tau^{\prime}\right) d \tau^{\prime}}{\tau}
$$

A correction coefficient linearly linking the cross section correction to the historical density change is defined as:

Historical moderator density correction : $S_{i\left[\mathrm{~cm}^{2} / \mathrm{g}\right]} \equiv \frac{\Delta \Sigma_{i}}{\rho(\vec{r}, \tau)-\rho_{H_{2} O}^{r e f}}$
Coefficient $S_{i}$ is computed for each cross section type using a depletion calculation, carried out at a different operating point by changing the water density. This type of correction makes unfortunately the coefficient $S_{i}$ having a physical dimension. We can get rid of this problem by another definition of the coefficient $S_{i}$ (as used in $E D F$ ), such as:

$$
\frac{\Sigma_{i}-\Sigma_{i, r e f}}{\Sigma_{i, r e f}} \equiv S_{i[-]} \times \frac{\rho(\vec{r}, \tau)-\rho_{H_{2} O}^{r e ́ f}}{\rho_{H_{2} O}^{r e ́ f}}
$$

It has been observed that in practice, this approach is highly reliable for operating points close to the nominal values. Such corrections may be neglected if the isotopic depletion is computed and the macroscopic cross section is deduced using the concentrations obtained through the depletion calculation:

[^338]$$
\Sigma_{i}=\sum_{j=1}^{N} N_{j} \sigma_{i}^{j}
$$

Nonetheless, it should be noted that the microscopic cross sections also depend on the concentrations of other isotopes. Further, these cross sections are very rarely tabulated in terms of isotopic composition given the high dimension of the required tabulation space. In this case, a microscopic cross section model is required, coupled with the use of a macroscopic feedback parameter such as a spectrum index. Thorough analyses of this phenomenon have shown that $90 \%$ of the effect on cross sections is due to isotopic concentrations. In addition, the leakage effects remain regardless of the model used, since the cross sections are not homogenized using the true core buckling. This effect is worth 200 pcm discrepancies on core calculations.

### 16.6 Historical Isotopic Correction

In the previous paragraphs, the historical isotopic effect in the Lefebvre-Seban model through the use of historical densities was described. Where there is a core code with an isotopic depletion module, the macroscopic cross sections are generally computed using a residual cross section and the microscopic cross sections of the $n$ isotopes considered in the microscopic depletion (henceforth called microisotopes):

$$
\Sigma_{a}^{C R N}=\Sigma_{a}^{r e s}+\sum_{i=1}^{n} N_{i} \sigma_{a}^{i}
$$

To obtain the spectral effect caused by a single isotope, for which the reference concentration is not known, the partial derivatives $\partial \sigma_{a}^{i} / \partial N_{j}$ and $\partial \Sigma_{a}^{r e s} / \partial N_{j}$ must be calculated for all micro-isotopes $j$, as well as the residual cross section (absorption, fission, etc.). This can be very onerous since several branch calculations are needed around each reference state point in the phase space. The reference depletion calculation as a function of burn-up is a "characteristic line" in the feedback phase space, and represents change in a neutron parameter (a cross section for instance). The branch calculations are then viewed as the points in a feedback parameter grid:

The example described in Fig. 16.12 is a feedback grid where the water density and the moderator temperature (Doppler effect of the moderator cross sections only) are changed on the first grid ( $\pm 20 \%$ ). Uncoupling the effects of these two parameters results in linearizing the effects in the vicinity of the operating point. The central line is the nominal depletion calculation (i.e. computed at the nominal feedback parameter values) with burn-up. The spectral effect inevitably leads to the
fact that depleting the fuel from the initial burn-up at non-nominal parameter values (for example $\left(T_{\bmod }^{0}-20 \%, \rho_{\bmod }^{0}+20 \%\right)$ ) will deviate in relation to the state point in the corresponding grid. This deviation is quantified graphically by the arrow $\mathbb{i}$. Similarly, the grids for other feedback parameters may be represented (Fig. 16.12).

The spectral-isotope technique (Marguet, developed in 2009) is a simple and efficient approach: it consists in introducing a pseudo-isotope, which is characteristic of the spectral effects due to the historical isotopic effect. Assuming that all micro-isotopes are absorbing, the absorption spectral effect of these isotopes may be summarized through a spectral-isotope $N^{*}$, created by weighting the reaction rates of all the micro-isotopes per energy group ( $G$ groups in the core calculation):

$$
\sigma_{a}^{*} N^{*} \Phi=\sum_{g=1}^{G} \sum_{i=1}^{n} N_{i} \sigma_{a, g}^{i} \Phi_{g}
$$

Supposing that only captures are important for the historical effects, the cross section of the spectral-isotope is modeled using a $1 / v$ law and an arbitrary cross section of $\sigma_{2200 \mathrm{~m} / \mathrm{s}}=1$ barn. The spectral-isotope concentration in the core code can thus be computed. The feedback effect of the spectral-isotope is obtained through an additional dimension (which is unique so as to avoid a large number of branch calculations) in the feedback phase space. In practice, this is done with the lattice code by changing the concentration of the absorbing isotope as $1 / v$. Hence, the differential feedback coefficients $\partial \sigma_{a}^{i} / \partial N^{*}$ and $\partial \Sigma_{a}^{\text {res }} / \partial N^{*}$ are obtained. For the other grid points not on the $N^{*}$ axis, it may be assumed that $N^{*}$ is equal to the reference value $N^{* 0}$ (this is not completely accurate if the definition of $N^{*}$ is considered, since the values of the other parameters in the branch calculations modify the $\sigma_{a, g}^{i}$, which are used in the weighting formula). To avoid setting any


Fig. 16.12 Branch calculations in the feedback phase space
hypothesis on the spectral-isotope, the branch calculations are computed using the microscopic reaction rates $\sigma_{a}^{*} N^{*} \Phi$ as the feedback parameter. The approach can be enhanced by creating a spectral-isotope for each energy group in the core calculation. Such a model effectively takes into account both the historical isotopic effect (especially the deviation in concentration) and the cooling effects for a reactor shutdown (e.g. americium-241 build-up). In conclusion, regarding the spectralisotope calculation, it may be useful to choose only those isotopes that undergo significant concentration changes with respect to feedback conditions while disregarding those highly correlated with burn-up such as ${ }^{235} U$ and ${ }^{238} U$.

## Chapter 17 <br> Reactor Kinetics

The goal of reactor physics is to maintain the reactor in a stable state. Nevertheless, the reactor must be brought to a stable state at full power, starting from a cold shutdown state. Further, a reactivity incident may modify the stable state thus achieved. Reactor kinetics studies the transient time phenomena and is the starting point of studies for reactivity accidents.
(Akcasu et al. 1971; Ash 1979; Bell and Glasstone 1970; Hetrick 1993; Keepin 1965; Planchard 1995, p. 215; Ott and Neuhold 1985; Rozon 1992; Soodak 1962, p. 248; Tellier 1993; Weaver 1963, 1964, 1968)

### 17.1 Prompt Neutrons

The starting hypothesis is that fission neutrons are emitted instantaneously as the incident neutron is absorbed. The emitted neutrons are said to be prompt neutrons, with a prompt emission spectrum (e.g. a Watt spectrum). Wigner proposed a didactic space-time representation of the fission phenomenon (Fig. 17.1):

0 A neutron, usually at thermal energy, in a water-moderated reactor, collides with a heavy nucleus.
1 The heavy nucleus is excited and splits up, just as a water droplet would be cut in two (liquid drop model).
2 The two fragments spread apart from one another, taking with them a considerable amount of the energy released by fission in the form of kinetic energy (approximately 170 MeV ).
3 Prompt neutrons are emitted ( $\approx 99 \%$ of neutrons are emitted within $10^{-14} \mathrm{~s}$ of fission). Two or three prompt fast neutrons are emitted.
4 Prompt $\gamma$ rays are emitted ( $\approx 7 \gamma$ rays).
5 The medium significantly slows down the fission fragments, and this phenomenon is more extensive if the density of the medium, $\rho$, is high. All the kinetic energy is then transformed into heat.


Fig. 17.1 The Wigner diagram describing fission

### 17.1.1 Evolution of a Hypothetical Prompt Neutron Reactor

A purely theoretical reactor is considered, in which the neutron population is multiplied only by prompt neutrons. The diffusion equation describing the neutron flux $\Phi$ for one energy group is expressed as:

with $D_{[\mathrm{cm}]}$ the diffusion coefficient and $\Sigma_{a\left[\mathrm{~cm}^{-1}\right]}$ the macroscopic absorption cross section. The flux is defined as $\Phi \equiv n v$, and hence, the neutron density change (specifying the nature of the source term) is written as:

$$
\frac{1}{v} \frac{\partial \Phi}{\partial t}=D \Delta \Phi-\Sigma_{a} \Phi+\overbrace{\underbrace{S_{f}}_{\text {Fission source }}+\underbrace{S_{d}}_{\begin{array}{c}
\text { Other sources } \\
(\text { at start }-u p)
\end{array}}}^{\text {Sources }}
$$

The multiplication factor in an infinite medium is expressed as:

$$
k_{\infty} \equiv \frac{\text { production }}{\text { absorption }}=\frac{\nu \Sigma_{f}}{\Sigma_{a}}
$$

Given $L$, the length of thermal diffusion, usually in cm :

$$
L_{[c m]} \equiv \sqrt{\frac{D}{\Sigma_{a}}} \text { or }: \quad L^{2} \equiv \frac{D}{\Sigma_{a}}
$$

The quantity $S_{f}$ represents the fission sources. $S_{d}$ represents the sources at the reactor start-up, such as a californium source placed at the center of the reactor for divergence and removed soon after. The amount of neutrons absorbed at thermal energy for a given generation is $\Sigma_{a} \Phi$. In an infinite medium, $k_{\infty} \Sigma_{a} \Phi$ new thermal neutrons are available for the next generation, i.e. $\nu \Sigma_{f} \Phi$ neutrons (Fig. 17.2).

The fission source term is given by $S_{f}=k_{\infty} \Sigma_{a} \Phi$. Thus:

$$
\frac{1}{v} \frac{\partial \Phi}{\partial t}=D \Delta \Phi+\left(k_{\infty}-1\right) \Sigma_{a} \Phi
$$

Which, when divided by the absorption cross section $\Sigma_{a}$ on both sides, becomes:

$$
\frac{1}{\Sigma_{a} v} \frac{\partial \Phi}{\partial t}=L^{2} \Delta \Phi+\left(k_{\infty}-1\right) \Phi
$$

In a finite reactor, the non-leakage probability of the geometrical design should be taken into accounted for (Fig. 17.3).

In a finite reactor, neutrons can disappear by absorption during slowing-down, as in an infinite medium (resonance escape probability factor $p$ ), by fast leakage from the epithermal finite lattice (non-leakage factor $e^{-B_{g}^{2}} \tau_{l h}$ where $B_{g}$ is the geometrical buckling of the reactor and $\tau_{t h}$ the thermal Fermi age) and by thermal leakage, which will be implicitly taken into account by solving the diffusion equation with zero flux at the extrapolated surface. $e^{-B_{g}^{2} \tau_{t h}}$ is the non-leakage probability of the reactor in the presence of absorption in the fast and epithermal energy range; $p$ is the resonance escape probability during slowing-down. Thus, the fission source is:

Fig. 17.2 Diagram showing the neutron balance between two generations of thermal neutrons



Fig. 17.3 Reactor of finite volume (here a cylindrical reactor)

$$
S_{f}=k_{\infty} \Sigma_{a} \Phi e^{-B_{g}^{2} \tau_{t h}}
$$

The flux equation is written as: $\frac{1}{v} \frac{\partial \Phi}{\partial t}=D \Delta \Phi+\Sigma_{a} \Phi\left(k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1\right)$
Or, alternatively: $\frac{1}{\Sigma_{a} v} \frac{\partial \Phi}{\partial t}=L^{2} \Delta \Phi+\left(k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1\right) \Phi$
$\ell_{[s]}$ is the time interval designating the mean neutron lifetime between the release of a neutron and its loss in the reactor. This time corresponds to the time of slowingdown and then the diffusion of a neutron before it is lost by sterile or fertile capture, or a new fission reaction. Assuming that the reactor is infinite, this time period is denoted as $\ell_{B_{g}=0}$ which, as will be seen later, is modified by neutron leakage at any energy (characterized by $e^{-M^{2} B_{g}^{2}}$ ), which modifies the neutron lifetime. The fact that the reactor is finite in space decreases the average neutron lifetime, whereas a reactor with a reflector will provide neutrons with a longer lifetime. Given that $n / \ell_{0}$ is the number of thermal neutrons lost per unit time in an infinite reactor, it is assumed that the neutrons are re-emitted instantaneously after absorption of the incident neutrons. Hence, $k_{\infty} n / \ell_{0}$ is the number of neutrons released at the new generation by the loss of $n / \ell_{0}$ neutrons. Thus, the balance is (Weaver 1963, p. 35):

$$
\frac{\Delta n}{\Delta t}=k_{\infty} \frac{n}{\ell_{0}}-\frac{n}{\ell_{0}}
$$

which is expressed as a continuous time derivative thus:

$$
\frac{d n}{d t}=\frac{k_{\infty}-1}{\ell_{0}} n
$$

Hence, the exponential growth law:

Exponential growth law for prompt neutrons in an infinite lattice:

$$
\begin{equation*}
n(t)=n(0) e^{\left(\frac{k_{\infty}-1}{\ell_{0}}\right) t} \tag{17.1}
\end{equation*}
$$

An exponential growth law for the neutron population is obtained. The latter increases when $k_{\infty}$ increases or the neutron lifetime decreases. This behavior is known as prompt over-critical (prompt subcritical respectively if $k_{\infty}<1$ ) since only prompt fast neutrons lead to neutron multiplication. The average neutron lifetime in an infinite lattice is given by:

Prompt neutron lifetime in an infinite lattice: $\ell_{0} \equiv \frac{\bar{\lambda}}{\mathrm{v}}=\frac{1}{\mathrm{v} \Sigma_{a}}$
where $\bar{\lambda}$ is the average absorption length (the mean distance travelled by a neutron in an erratic way before its absorption, including scattering), and $v$ is the mean velocity of the neutrons. $\ell_{0}$ is the average time interval between the birth of the neutron by fission and its loss, usually at thermal state, by absorption [the notations here are the same as those of (Glasstone and Edlund 1972)]. It is inversely proportional to the macroscopic absorption cross section (if the medium is more abundant, the neutron has a lower chance of survival). In a reactor with natural uranium, this time is of the order of $10^{-3} \mathrm{~s}$, but this decreases to $10^{-4} \mathrm{~s}$ in a reactor with enriched uranium. The velocity used in this formula is the mean neutron velocity in the reactor (and not that of fast neutrons), assuming that the slowingdown time is differentiated from the scattering time. In a finite reactor, the non-leakage probability of the medium must be multiplied by $\ell_{0}$ to account for leakage (Kahan and Gauzit 1957, p. 167). Thus:

Prompt neutron lifetime in an infinite lattice: $\quad \ell_{B_{g}}=\frac{\ell_{0}}{1+L^{2} B_{g}^{2}}$
For larger piles, in which there is a smaller degree of geometrical buckling, this effect may be disregarded. The term average neutron generation time, also called the neutron renewal period, is defined by some authors, (Lewins 1978, p. 57) as the mean time for a neutron to produce a new generation of neutrons ${ }^{1}$ :

Prompt neutron generation time: $\quad \ell \equiv \frac{1}{\mathrm{v} \nu \Sigma_{f}}$
Nonetheless, the notion of neutron generation time can be ambiguous if a precise physical meaning is attached to it. The mean free path is defined as:

[^339]$$
\lambda_{t}=\int_{0}^{+\infty} x e^{-\Sigma_{t} x} \Sigma_{t} d x=\frac{1}{\Sigma_{t}}
$$

It is the average distance travelled between two collisions given that $e^{-\Sigma_{t} x}$ is the non-collision probability for path $x$. The time $\ell_{t}=\lambda_{t} / v$ is the mean time between two collisions in which the neutron travels part of a straight line. The mean free (collision-free) path of absorption (capture, fission or scattering respectively) is the average distance between the emission of the neutron and its absorption after the first collision. It is expressed as:

$$
\lambda_{a}=\int_{0}^{+\infty} x e^{-\Sigma_{t} x} \Sigma_{a} d x=\frac{\Sigma_{a}}{\Sigma_{t}^{2}}=\frac{\Sigma_{a}}{\Sigma_{t}} \lambda_{t}
$$

(resp. $\lambda_{c}=\Sigma_{c} \lambda_{t} / \Sigma_{t}, \lambda_{f}=\Sigma_{f} \lambda_{t} / \Sigma_{t}$ or $\lambda_{s}=\Sigma_{s} \lambda_{t} / \Sigma_{t}$ ). Indeed, the absorption of a neutron supposes that there has been no previous interaction, meaning that the neutron travels in a straight line until it is absorbed (is captured, induces fissions or is scattered, respectively). These distances are the product of the mean free path and the considered reaction probability, and they have an additive property such that:

$$
\lambda_{t}=\lambda_{a}+\lambda_{s}=\lambda_{f}+\lambda_{c}+\lambda_{s}
$$

If these mean free paths are divided by the velocity, the mean free times of flight are obtained, which are also additive. The mean free absorption path can be computed by weighing path $x$ by the non-absorption probability $e^{-\Sigma_{a} x}$ (but scattering is possible), then by the absorption probability on the path $d x$ (hence, $\Sigma_{a} d x$ ):

$$
\overline{\lambda_{a}}=\int_{0}^{+\infty} x e^{-\Sigma_{a} x} \Sigma_{a} d x=\frac{1}{\Sigma_{a}}
$$

Dividing this mean path by the velocity gives the average time between emission and absorption. This can also be applied to the mean fission path (average distance between emission and fission in a non-straight line) and for capture (average distance between emission and capture in a non-straight line):

$$
\overline{\lambda_{f}}=\int_{0}^{+\infty} x e^{-\Sigma_{a} x} \Sigma_{f} d x=\frac{\Sigma_{f}}{\Sigma_{a}^{2}} \text { and } \overline{\lambda_{c}}=\int_{0}^{+\infty} x e^{-\Sigma_{a} x} \Sigma_{c} d x=\frac{\Sigma_{c}}{\Sigma_{a}^{2}}
$$

and not $1 / \Sigma_{f}$ or $1 / \Sigma_{c}$ as might be expected. It should be noted from the above that $1 /\left(\Sigma_{f} v\right)$ is not the mean time between emission and fission (resp. $1 /\left(\Sigma_{c} v\right)$ for capture) since, using the respective mean free paths, $\ell_{f}=\Sigma_{f} /\left(\Sigma_{a}^{2} v\right)$ and $\ell_{c}=\Sigma_{c} /\left(\Sigma_{a}^{2} v\right)$ are
obtained. Furthermore, the lack of physical meaning of the length in terms of mean path makes physical interpretation of the neutron generation time risky. Some authors see it as the neutron generation time normalized to one neutron produced by sheer intellectual construction. ${ }^{2}$ I personally prefer to see only a definition in the neutron generation time: $\ell \equiv \ell_{B_{g}} / k_{\text {eff }}$.

Numerical example: Given a thermal neutron reactor with the following properties: $\Sigma_{a}=0.076 \mathrm{~cm}^{-1}, D=0.21 \mathrm{~cm}, B_{g}^{2}=0.01 \mathrm{~cm}^{2}$. In a thermal Maxwell spectrum at $20.44{ }^{\circ} \mathrm{C}(293.59 \mathrm{~K})$ where $v_{0}=2200 \mathrm{~m} . \mathrm{s}^{-1}$, the mean velocity is given by:

$$
\bar{v}=\frac{2}{\sqrt{\pi}} \sqrt{\frac{T}{T_{0}}} v_{0}=2480 \quad \mathrm{~m} \cdot \mathrm{~s}^{-1}
$$

where the prompt neutron lifetime in an infinite lattice of the order of $50 \mu \mathrm{~s}$ : $\ell_{0}=5.3 \times 10^{-5} \mathrm{~s}$ and $\ell_{B_{g}}=5.16 \times 10^{-5} \mathrm{~s}$ for a $P W R$. This value should be compared with those of Natural Uranium Graphite Gas (UNGG) reactors, of the order of $10^{-2}-10^{-3} \mathrm{~s}$, and of fast neutron reactors, at $10^{-6} \mathrm{~s}$. The exponential growth law leads to a $k_{\text {eff }}$ of 1.00100 ( 100 for 100,000 in reactivity) with $n(t) \approx n(0) e^{20 t}$. In this case, with just 100 pcm of over-criticality (very slightly more than 10 ppm of natural boron in the moderator, the same order of magnitude as the uncertainty of measure of boron in a reactor), the neutron population "explodes" due to the 20 in the exponential term, making the reactor virtually uncontrollable by any method known to man. The reactor period, $T$, which corresponds to the time period in which the neutron population is multiplied by $e$, is given by:

Prompt period of infinite reactor: $T=\frac{\ell_{0}}{k_{\infty}-1}$
which for a 100 pcm of reactivity: $T \approx 0.05 \mathrm{~s}$. This is not technologically viable, since no automatic system or human action can possibly counteract such a surge in power.

### 17.1.2 Flux Calculation: Point Reactor Hypothesis

The mean neutron lifetime in an infinite lattice (the 0 index is for geometrical buckling of zero) $\ell_{0} \equiv 1 /\left(\Sigma_{a} v\right)$ appears in the flux equation:

[^340]$$
\ell_{0} \frac{\partial \Phi}{\partial t}=L^{2} \Delta \Phi+\left(k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1\right) \Phi
$$

The hypothesis (not always verified!) that the space and time variables are separable is applied:

$$
\Phi(\vec{r}, t)=\varphi(\vec{r}) \Psi(t)
$$

This principle consists in assuming that the time variation of the flux is homogeneous in space, which has been known for obscure historical reasons in English as the "point-kinetic model". This can lead to the erroneous assumption that a 0D hypothesis is being applied (this particular model will be studied later). This factorization of the flux is inserted in the diffusion equation:

$$
\ell_{0} \varphi(\vec{r}) \frac{d \Psi(t)}{d t}=L^{2} \Psi(t) \Delta \varphi(\vec{r})+\left(k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1\right) \varphi(\vec{r}) \Psi(t)
$$

The time variables are grouped on the LHS of the equation and the space variables on the RHS to give:

$$
\frac{\ell_{0}}{\Psi(t)} \frac{d \Psi(t)}{d t}=\frac{L^{2} \Delta \varphi(\vec{r})}{\varphi(\vec{r})}+k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1
$$

Close to criticality, the spatial shape of the flux $\varphi(\overrightarrow{\mathrm{r}})$ obeys (at first-order approximation) to a fundamental mode-this is the second approximation of the point kinetics model:

$$
\Delta \varphi(\vec{r})+B_{g}^{2} \varphi(\vec{r})=0
$$

where:

$$
\frac{\ell_{0}}{\Psi(t)} \frac{d \Psi(t)}{d t}=k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1-L^{2} B_{g}^{2}
$$

Dividing by $1+L^{2} B_{g}^{2}$, the following can be expressed: $k_{e f f}=\frac{k_{\infty}}{1+L^{2} B_{g}^{2}} e^{-B_{g}^{2} \tau_{t h}}=\frac{k_{\infty}}{1+M^{2} B_{g}^{2}}$
where:

$$
k_{e f f}-1=\frac{\ell_{0}}{1+L^{2} B_{g}^{2}} \frac{1}{\Psi(t)} \frac{d \Psi(t)}{d t}
$$

By denoting the prompt neutron lifetime in an infinite medium as: $\ell_{B_{g}} \equiv \frac{\ell_{0}}{1+L^{2} B_{g}^{2}}$, the following is obtained:

$$
\frac{d \Psi(t)}{d t}=\frac{k_{e f f}-1}{\ell_{B_{g}}} \Psi(t)
$$

Using $\Phi(\vec{r}, 0)=\varphi(\vec{r}) \Psi(0)=$ Cst $\varphi(\vec{r})$, finally, the following can be written:

$$
\Phi(\vec{r}, t)=\Phi(\vec{r}, 0) e^{\frac{k_{e f f}-1}{\ell_{B_{g}}}} t
$$

By calculation, the following growth law is obtained: $n(t)=n(0) e^{\frac{k_{\text {eff }}-1}{\ell_{B}}} t$, with $\Phi \equiv n v$ found as usual.

Returning to the previous numerical example and using the reactivity $\rho \equiv\left(k_{\text {eff }}-1\right) / k_{\text {eff }}$ expressed in pcm (pour cent mille—literally "per 100,000"), a 100 pcm increase in reactivity (as seen in Fig. 17.4), $\left(\rho \approx k_{\text {eff }}-1\right.$ when $k_{\text {eff }}$ is close to 1) leads to exponential behavior of the flux: $k_{\text {eff }}=1.001, \rho \approx 100 \mathrm{pcm}, \Phi(\vec{r}, t) \approx$ $\Phi(\vec{r}, 0) e^{20}{ }^{t}$ (Fig. 17.5).

Under these conditions, the reactor is uncontrollable. Fortunately, this simplified approach does not account for a fraction of neutrons emitted a certain time after fission, i.e. deferred or delayed neutrons, which play a pivotal role in the stability of the reactor.

### 17.2 Delayed Neutrons

After the discovery of fission in 1939, Roberts, Hafstad, Meyer and Wang observed the emission of deferred neutrons, ${ }^{3}$ sometimes several dozen seconds after fission. Roberts and his team bombarded a uranium nitrate bottle with a beam of deuterium. Using an ionization chamber with a boron deposit, they detected the presence of neutrons up to 2 min after the end of irradiation. Two possible explanations were put forward: either direct disintegration of certain fission products emitting neutrons or photodisintegration emitting high-energy photons, a solution that was later rejected (Figs. 17.6 and 17.7, Photo 17.1).

This phenomenon was explained by Niels Bohr and John A. Wheeler ${ }^{4}$ as the result of a nuclear excitation, followed by $\beta^{-}$decay of the fission fragments. Well before sustained chain reactions were being considered, the importance of deferred neutrons to control the reaction was understood. The basic mechanism is as follows: in some cases, fission of a heavy nucleus produces a fission product far from the stable-isotope region. One of the two fragments has an excess of neutrons. Most

[^341]Fig. 17.4 Reactivity
Heaviside step function

Fig. 17.5 Evolution of the flux in an over-critical prompt reactor

Fig. 17.6 Production of deferred neutrons by fission

Fig. 17.7 Production of delayed neutrons by fission





Photo 17.1 John Wheeler (Pinceton)


Fig. 17.8 Wigner representation of fission with delayed neutrons
0 to 5 As for emission of prompt neutrons
6 One of the fission products has a large excess of neutrons and decays with $\beta^{-}, n$ (emission of an electron and a neutron). In the above diagram, the other fission product is assumed to be stable
fission products are $\beta^{-}$-radioactive but some isotopes with a large excess of neutrons can also be $\beta^{-}, n$ (a phenomenon also known as neutron decay). This is possible if the isotope is in an excited state above the binding energy of the neutron to the daughter isotope. The neutron decay period is that of the isotope with a neutron excess, known as a precursor. Figure 17.8 shows the Wigner representation of fission, with the deferred neutrons added. The latter are emitted in small quantities but with significant delay with respect to the initial absorption for prompt neutrons. This delay modifies the average neutron lifetime significantly as will be shown next.

A common mistake is to assume that since delayed neutrons are produced in small quantities when normalized to one fission, their effect can be disregarded. This is not the case at all, since most neutrons in a reactor are, in fact, "hidden" in the precursors, concentrations of which are 1000 greater than the effective neutron density. The precursors are somewhat equivalent to a reservoir or buffer stock of neutrons for the core.

This is due to the fact that the radioactive periods of precursors can be very long compared to the life of the prompt neutrons, thereby increasing the mean neutron generation time.

Given the particular fission case: ${ }_{0}^{1} n+{ }_{92}^{235} U \rightarrow{ }_{35}^{87} \mathrm{Br}+{ }_{57}^{147} \mathrm{La}+{ }_{0}^{1} n+{ }_{0}^{1} n$, bromine 87 is radioactive with $\beta^{-}$decay having a period of 55.7 s :

$$
{ }_{35}^{87} B r \rightarrow{ }_{36}^{87} K r^{*}+{ }_{-1}^{0} e^{-}
$$

The resulting krypton 87 has a large excess of neutrons and decays almost instantaneously according to two modes (Fig. 17.9):


Fig. 17.9 Decay scheme of Bromine 87

$$
{ }_{36}^{87} \mathrm{Kr}^{*} \rightarrow\left\{\begin{array}{l}
{ }_{36}^{86} \mathrm{Kr}+{ }_{0}^{1} n \quad(2.9 \%) \\
{ }_{37}^{87} \mathrm{Rb}+{ }_{-1}^{0} e^{-} \quad(97.1 \%)
\end{array}\right.
$$

Hence, Bromine ${ }_{35}^{87} \mathrm{Br}$ is a precursor for delayed neutrons. As a fission product, ${ }_{35}^{87} B r$ is produced with a yield depending on the energy of the incident neutron and the fissile nucleus. Other precursors have been identified, and the particular case of iodine ${ }_{53}^{137} I$ with period 22.72 s should be noted.

$$
{ }_{53}^{137} I \rightarrow{ }_{54}^{137} X e^{*}+{ }_{-1}^{0} e^{-} \text {then }{ }_{54}^{137} X e^{*} \rightarrow{ }_{54}^{136} X e+{ }_{0}^{1} n
$$

Let $\beta_{i}$ be the number of deferred neutrons emitted by the fission product i (precursor) after a fission, and $\lambda_{i}$ the decay constant of the precursor. The value of $\beta_{i}$ depends on the heavy fissile nucleus and the energy of the incident neutrons (hence, the spectrum of neutrons in the reactor). $\beta_{i}$ is expressed in pcm (the number of deferred neutrons is very small) of the total amount of neutrons emitted by fission. For ${ }_{35}^{87} \mathrm{Br}$ in the reaction $\left({ }_{92}^{235} U+n\right)_{\text {thermal }}, \beta_{35}^{87} B r=21 \mathrm{pcm}$. This is equivalent to $21 \times 10^{-5}$ neutrons emitted with a period of 55.7 s for one emitted neutron. Historically, delayed neutrons were grouped into six precursor families (it was long thought that only six fission products emitted delayed neutrons. In fact, there are about a hundred of them). Recent developments have led to a finer description with eight families. An exhaustive compilation of kinetic data is given in Tuttle (Table 17.1). ${ }^{5}$

### 17.2.1 Delayed Neutron Fraction

The delayed neutron yield is the number of delayed neutrons brought to one fission such that $n_{d} / F$. The total delayed neutron fraction $\beta$, i.e. the sum over all delayed neutron fractions for precursors of delayed neutrons, is equal to the ratio between the delayed neutron yield $n_{d} / F$ and the number of neutrons emitted by fission, $\bar{\nu}$ :

Delayed neutron fraction: $\beta \equiv \sum_{i \in\{\text { precursor }\}} \beta_{i} \quad \beta \equiv \frac{\frac{n_{d}}{F}}{\bar{\nu}}$
Each precursor family groups the precursors with similar periods. A mean period is associated with each family. The latter is computed as the average period for $\left(\beta^{-}, n\right)$ decays for precursors in the family. The families are generally called delayed neutron groups, which should not be confused with the energy groups in a calculation discretized in energy (Tables 17.2 and 17.3).

[^342]Table 17.1 Delayed neutron fractions for fast and thermal incident neutrons

| Heavy nucleus | Fast fission |  |  | Thermal fission |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\frac{n_{d}}{F}$ | $\bar{\nu}$ | $\beta$ | $\frac{n_{d}}{F}$ | $\bar{\nu}$ | $\beta$ |
| ${ }_{94}^{241} P u$ | - | - | - | 0.0154 | 3.14 | 0.00490 |
| ${ }_{94}^{240} \mathrm{Pu}$ | 0.0088 | 3.3 | 0.00260 | - | - | - |
| ${ }_{94}^{239} \mathrm{Pu}$ | 0.0063 | 3.09 | 0.00200 | 0.0061 | 2.87 | 0.00210 |
| ${ }_{92}^{238} U$ | 0.0412 | 2.79 | 0.01480 | - | - | - |
| ${ }_{92}^{235} U$ | 0.0165 | 2.57 | 0.00640 | 0.0158 | 2.43 | 0.00650 |
| ${ }_{92}^{233} U$ | 0.0070 | 2.62 | 0.00260 | 0.0066 | 2.48 | 0.00260 |
| ${ }_{90}^{232} \mathrm{Th}$ | 0.0496 | 2.44 | 0.02030 | - | - | - |

Non-fissile systems at the considered energy are not given here

Table 17.2 Kinetic data for six precursor groups

| Group | $T$ | $\lambda$ | ${ }_{92}^{235} U+n_{\text {th }}$ | ${ }_{94}^{239} P u+n_{\text {th }}$ | ${ }_{92}^{233} U+n_{\text {th }}$ |
| :--- | :--- | :--- | :---: | :---: | :---: |
| $1\left({ }_{35}^{87} B r\right)$ | 55.7 | 0.0124 | 21 | 7 | 23 |
| $2\left({ }_{53}^{17} I\right)$ | 22.72 | 0.0305 | 142 | 63 | 79 |
| 3 | 6.22 | 0.111 | 128 | 45 | 67 |
| 4 | 2.30 | 0.301 | 257 | 69 | 74 |
| 5 | 0.61 | 1.14 | 75 | 18 | 14 |
| 6 | 0.23 | 3.01 | 27 | 9 | 9 |
| $P c m$ |  |  | 650 | 210 | 270 |

Table 17.3 Effect of incident neutron energy on kinetic parameters of certain fissile systems

| Neutron <br> energy | Fissile <br> isotope | Delayed neutron <br> yield per fission | $\nu$ number of <br> neutrons per <br> fission | $\beta$ delayed <br> neutron <br> fraction | $\lambda=\frac{\beta}{\lambda}$$\sum_{\{\text {precursor }\}} \frac{\beta_{i}}{\lambda_{i}}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 0.0253 eV | ${ }_{92}^{235} U$ | 0.0158 | 2.432 | 0.00650 | 0.0767 |
| 0.0253 eV | ${ }_{94}^{239} P u$ | 0.0061 | 2.874 | 0.00212 | 0.0648 |
| 0.0253 eV | ${ }_{92}^{233} U$ | 0.0066 | 2.482 | 0.00266 | 0.0543 |
| 1.45 MeV | ${ }_{92}^{235} U$ | 0.0165 | 2.570 | 0.00642 | 0.0784 |
| 1.58 MeV | ${ }_{94}^{239} \mathrm{Pu}$ | 0.0063 | 3.090 | 0.00204 | 0.0683 |
| 1.45 MeV | ${ }_{92}^{233} U$ | 0.0070 | 2.620 | 0.00267 | 0.0559 |

After Hetrick (1993)

### 17.3 Effect of Delayed Neutrons on Reactor Kinetics

As seen previously, if all the neutrons emitted by fission were prompt, the reactor would not be controllable. Given $\theta_{i}$ the mean lifetime of precursor $i$ (henceforth, the precursor group will be simply denoted as precursor). The neutrons emitted by the precursor appears after a time period of $\theta_{i}$. The mean delay of the group is then $\beta_{i} \theta_{i}$.

Therefore, intuitively, the mean thermal neutron generation lifetime is no longer $\ell_{0}$ as in the hypothetical case in which all neutrons were prompt. In fact, it is the average of the prompt lifetime and the deferred lifetime $\bar{\ell}$ defined as:

$$
\bar{\ell}=\ell_{0}+\sum_{i} \beta_{i} \theta_{i}
$$

The mean lifetime $\theta_{i}$ of an isotope of period $T_{i}$ (corresponding to the decay constant $\lambda_{i}$ ) is the time in which the number of nuclei is divided by the Neper constant $e$ :

$$
\theta_{i}=\frac{1}{\lambda_{i}}
$$

This result can be obtained by considering that out of n neutrons emitted in the core, there are $n(1-\beta)$ prompt neutrons with mean lifetime and there are $n \beta$ delayed neutrons. Since $\theta=\sum_{i} \beta_{i} \theta_{i} / \beta$ is the mean lifetime of the precursors averaged over the precursor families, the mean lifetime of neutrons emitted by the precursors is:

$$
\ell_{0}+\theta=\ell_{0}+\sum_{i} \beta_{i} \theta_{i} / \beta
$$

The average, weighted by the number of neutrons for each type, leads to the generation time:

$$
n \bar{\ell}=n(1-\beta) \ell_{0}+n \beta\left(\ell_{0}+\sum_{i} \beta_{i} \frac{\theta_{i}}{\beta}\right)
$$

hence, the previous result:
Average of prompt anddelayed neutron lifetimes: $\bar{\ell}=\ell_{0}+\sum_{i} \beta_{i} \theta_{i}$
Applied to the system ${ }_{92}^{235} U+{ }_{0}^{1} n_{\text {thermal }}$ this leads to:

$$
\begin{aligned}
\sum_{i \leq 6} \beta_{i} \theta_{i} & =\left[21 \frac{1}{0.0124}+142 \frac{1}{0.0305}+128 \frac{1}{0.111}\right. \\
& \left.\times+257 \frac{1}{0.301}+75 \frac{1}{1.14}+27 \frac{1}{3.01}\right] \cdot 10^{-5} s \\
& =8.43 \quad 10^{-2} s
\end{aligned}
$$

Table 17.4 Fast neutron lifetimes in a moderator

| Moderator | Fast neutron lifetime(s) |
| :--- | :--- |
| Water | $2 \times 10^{-4}$ |
| Heavy water | 0.14 |
| Beryllium | $4 \times 10^{-3}$ |
| Graphite | $1.6 \times 10^{-2}$ |

From Glasstone and Sesonske (1994, p. 242)
Which is around 0.1 s . In a true $P W R$ spectrum, the lifetime of prompt neutrons in an infinite lattice is $\ell_{0} \approx 2 \times 10^{-5} \mathrm{~s}$, which significantly increases the mean lifetime of prompt and delayed neutrons:

$$
\bar{\ell}=\ell_{0}+\sum_{i \leq 6} \beta_{i} \theta_{i} \approx 2 \times 10^{-5}+8.4 \times 10^{-2} \text { where: } \bar{\ell} \approx 0.1 \mathrm{~s}
$$

The lifetime of prompt neutrons in a reactor is shorter than the lifetime of fast neutrons scattering off a pure moderator (Table 17.4) due to absorption by heavy nuclei.

Where $T$ is the reactor period (time interval after which the flux is multiplied by $e$ ):

$$
\Phi(\vec{r}, T)=e \Phi(\vec{r}, 0)=\Phi(\vec{r}, 0) e^{\frac{k_{\text {eff }}-1}{\bar{\ell}} T}
$$

Thus, the period of the real reactor is:
Period of real reactor: $\quad T=\frac{\bar{\ell}}{k_{\text {eff }}-1}$
If $\rho=100 \mathrm{pcm}=0.00100$, then $T \approx 100 \mathrm{~s}$, in contrast with the 0.05 s period obtained by assuming that the reactor contained only prompt neutrons. This is equivalent to saying that "the reactor is 2000 times less responsive". Practically, the multiplication factor can be decomposed into two terms:

$$
k_{e f f}=k_{e f f}(1-\beta)+k_{e f f} \beta
$$

In a reactor that can be controlled, $k_{\text {eff }}(1-\beta)$ is such that it is slightly under 1. Therefore, the increase in the number of neutrons is principally due to the term $k_{e f f} \beta$, i.e. the delayed neutrons. Where $k_{\text {eff }}(1-\beta)>1$, i.e. $k_{\text {eff }}>1 /(1-\beta) \approx 1+\beta$, the reactor will be over-critical only with prompt neutrons. The reactor is said to be prompt over-critical. This state is reached when a reactivity of $\rho=1-1 / k_{\text {eff }}=\beta$ is inserted, and it is amplified dangerously where $\rho>\beta$. The reactor quickly becomes uncontrollable, as shown in the numerical example for the prompt critical reactor. The unit of reactivity is the dollar (symbol $\$, 1 / 100$ of a $\$=1$ cent); although mysterious for the uninitiated public, this unit is simply the reactivity expressed in multiples of $\beta$. Hence, if $\beta=700 \mathrm{pcm}$ and $\rho=1400 \mathrm{pcm}$ are inserted, this is equivalent to the insertion of $2 \$$. The situation can be summed up as follows:

| $k_{\text {eff }}<1$ | The reactor is sub-critical. Starting from <br> a stable state, the power decreases. The <br> fission power fades out leaving only the <br> residual decay power due to fission <br> products |  | Power |
| :--- | :--- | :--- | :--- |
| $k_{\text {eff }}=1$ | The reactor is critical. Starting from a <br> stable state, the power remains constant |  |  |
| $1<k_{\text {eff }}<\frac{1}{1-\beta}$ | The reactor is delayed over-critical. <br> Starting from a stable state, the power <br> increases in a controllable manner |  |  |
| Power |  |  |  |

### 17.4 Neutron Kinetics Equation

The neutron balance at one energy group, as previously seen, is written as:

$$
\frac{\partial n(t)}{\partial t}=\frac{1}{v} \quad \frac{\partial \Phi}{\partial t}=D \Delta \Phi-\Sigma_{a} \Phi+S
$$

which, in the case of a start-up without an independent source, is:

$$
\frac{1}{v} \frac{\partial \Phi}{\partial t}=D \Delta \Phi+\left(k_{\infty}-1\right) \Sigma_{a} \Phi
$$

The term $k_{\infty} \Sigma_{a} \Phi$, which represents the neutron fission source, can be broken down into the production of prompt neutrons $(1-\beta) k_{\infty} \Sigma_{a} \Phi$ and of delayed neutrons $\beta k_{\infty} \Sigma_{a} \Phi=\sum_{i=1}^{6} \lambda_{i} C_{i}$, where $C_{i}$ is the precursor concentration. The precursor decay rate, given by:

$$
-\frac{d C_{i}}{d t}=\lambda_{i} C_{i}
$$

is equal to the rate of creation of deferred neutrons emitted by the precursor. The quantity $\sum_{i=1}^{6} \lambda_{i} C_{i}$ is, thus, the rate of appearance of delayed neutrons, irrespective of their origin.

Hence: $\quad k_{\infty}(1-\beta) \Sigma_{a} \Phi+\left(\sum_{i=1}^{6} \lambda_{i} C_{i}\right)-\Sigma_{a} \Phi+D \Delta \Phi=\frac{1}{v} \quad \frac{\partial \Phi}{\partial t}$
Assuming that the flux obeys the fundamental mode: $\quad \Delta \Phi+B_{g}^{2} \Phi=0$
The geometrical buckling can be introduced in the diffusion equation:

$$
\left(k_{\infty}(1-\beta)-M^{2} B_{g}^{2}-1\right) \Phi+\sum_{i=1}^{6} \frac{\lambda_{i} C_{i}}{\Sigma_{a}}=\frac{1}{v \Sigma_{a}} \frac{\partial \Phi}{\partial t}
$$

as well as the migration area:

$$
M^{2} \equiv \frac{\int_{0}^{\infty} D(E) \Phi(E) d E}{\int_{0}^{\infty} \Sigma_{a}(E) \Phi(E) d E}
$$

and the prompt neutron lifetime, which in an infinite lattice, is given by:
$\ell_{0} \equiv \frac{1}{v \Sigma_{a}}$ and in a finite medium by: $\ell_{B_{g}} \equiv \frac{1}{v \Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)}=\frac{\ell_{0}}{1+M^{2} B_{g}^{2}}$
Since:

$$
k_{e f f}=\frac{k_{\infty}}{1+M^{2} B_{g}^{2}}
$$

the following is obtained: $\left(k_{\text {eff }}(1-\beta)-1\right) \Phi+\sum_{i=1}^{6} \frac{\lambda_{i} C_{i}}{\Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)}=\ell_{B_{g}} \frac{\partial \Phi}{\partial t}$
by dividing the previous equation by $1+M^{2} B_{g}^{2}$. The neutron density equation is deduced since $\Phi(t)=n(t) v$ :

$$
\frac{\partial n(t)}{\partial t}=\frac{\left(k_{\text {eff }}(1-\beta)-1\right) n(t)}{\ell_{B_{g}}}+\sum_{i=1}^{6} \frac{\lambda_{i} C_{i}}{\ell_{B_{g}} v \Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)}
$$

If $\ell_{B_{g}}=\frac{1}{v \Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)}$ is inserted, the neutron kinetics equation is established:

Neutron kinetics equation: $\frac{\partial n(t)}{\partial t}=\frac{k_{e f f}(\rho-\beta)}{\ell_{B_{g}}} n(t)+\sum_{i=1}^{6} \lambda_{i} C_{i}$

### 17.4.1 Precursor Concentration

The precursor $C_{i}$ is assumed to be $100 \%$ radioactive fission product. The precursor is itself produced by fission of fissile atoms with a yield $\gamma_{i}$. The Bateman equation for these precursors is written as:


The number of delayed neutrons $n_{i}$ from the precursor $C_{i}$ is written as:


The radioactive decay of neutrons is due to the fact that the free neutron is naturally $\beta^{-}$radioactive with a period of 11 min . In practice, in most kinetic cases, the natural decay of neutrons is disregarded ( 11 min is more than 10 times greater than the longest period of delayed neutrons: ${ }_{35}^{87} \mathrm{Br}$ of period 55.7 s . Further, since the concentration of neutrons $n_{i}$ is negligible compared to $C_{i}$, it may legitimately be advanced that $\lambda_{n} n_{i} \ll \lambda_{i} C_{i} / 10000$ ). Furthermore, the loss and creation of precursors under neutron flux are also disregarded since the corresponding absorption cross sections are very small. The very definition of $\beta_{i}$ is equivalent to the number of delayed neutrons with respect to the total number of neutrons emitted:

$$
\beta_{i} \equiv \frac{\gamma_{i} \Sigma_{f} \Phi}{\nu \Sigma_{f} \Phi}=\frac{\gamma_{i}}{\nu}
$$

Substituting $\gamma_{i}$ in the expression of $\frac{\partial C_{i}}{\partial t}$, simplified under the previous hypotheses, the following is obtained:


If the precursor is not $100 \%$ radioactive with neutron decay (as for ${ }_{35}^{87} \mathrm{Br}$ where only $2.9 \%$ of decays produced a neutron), the branching ratio of neutron decay $B r_{i}$ must be taken into account in the formula for neutron production $n_{i}$ :

$$
\frac{\partial n_{i}}{\partial t}=+B r_{i} \lambda_{i} C_{i}-\beta_{i} k_{\infty} \Sigma_{a} \Phi
$$

Multiplication of the equation $\frac{\partial C_{i}}{\partial t}$ by $B r_{i}$ leads to:

$$
\frac{\partial\left(B r_{i} C_{i}\right)}{\partial t}=-\lambda_{i} B r_{i} C_{i}+B r_{i} \gamma_{i} \Sigma_{f} \Phi
$$

The rate of loss of $B r_{i} C_{i}$ is equal to the rate of creation of $n_{i}$ :

$$
\frac{\partial\left(B r_{i} C_{i}\right)}{\partial t}+\frac{\partial\left(n_{i}\right)}{\partial t}=0
$$

where: $\beta_{i} k_{\infty} \quad \Sigma_{a} \Phi=B r_{i} \gamma_{i} \Sigma_{f} \Phi$
Since, by definition, $k_{\infty} \equiv \frac{\nu \Sigma_{f} \Phi}{\Sigma_{a} \Phi}$ and $\beta_{i} \nu \equiv B r_{i} \gamma_{i}$, the following is obtained:

$$
\frac{\partial\left(B r_{i} C_{i}\right)}{\partial t}=-\lambda_{i}\left(B r_{i} C_{i}\right)+\beta_{i} k_{\infty} \Sigma_{a} \Phi
$$

Taking into account the decay branching ratio in the precursor concentration, the same equation is obtained as for the case in which the precursor is $100 \%$ radioactive with neutron decay. The quantity $B r_{i} C_{i}$ is the number of latent neutrons in the part of ${ }_{35}^{87} \mathrm{Br}$ (for example) that produces deferred neutrons. The precursor is not technically a fission product but rather the contribution of this fission to neutron production. In practice, this is often a source of confusion for many people.

### 17.4.2 Point-Reactor Kinetics

(Akcasu et al. 1971, p. 49)

The term point-reactor kinetics conveys the hypothesis that the flux can be factorized as a product of two functions, one dependent on time and the other on space (i.e. $\Phi(\vec{r}, t)=\varphi(\vec{r}) \Psi(t))$. In practical cases, the space-dependent function may also vary with time. To assume that it is constant over time intervals, it is recalculated for a next time step. Classically these equations are written as:

$$
\begin{gathered}
\frac{\partial n(t)}{\partial t}=\frac{(\rho-\beta)}{\ell_{B_{g}} / k_{e f f}} n(t)+\sum_{i=1}^{6} \lambda_{i} C_{i} \\
\frac{\partial C_{i}}{\partial t}=-\lambda_{i} C_{i}+\beta_{i} k_{\infty} \Sigma_{a} \Phi=-\lambda_{i} C_{i}+\beta_{i} k_{\infty} v \Sigma_{a} n(t) \\
=-\lambda_{i} C_{i}+\beta_{i} k_{e f f}\left(1+M^{2} B_{g}^{2}\right) v \Sigma_{a} n(t)
\end{gathered}
$$

The following can be written: $\frac{\partial C_{i}}{\partial t}=-\lambda_{i} C_{i}+\frac{\beta_{i} k_{\text {eff }}}{\ell_{B_{g}}} n(t)$
where, by denoting $\ell \equiv \ell_{B_{g}} / k_{\text {eff }}$ the effective lifetime of prompt neutrons, also called the neutron generation time (Hetrick 1993, p. 10), the classical equations from all books on neutron kinetics (Hetrick 1993; Keepin 1965; Ott and Neuhold 1985; Rozon 1992; Tellier 1993) are obtained:

Point-reactor kinetics equations with 6 groups of delayed neutrons:

$$
\left\{\begin{array}{l}
\frac{\partial n(t)}{\partial t}=\frac{(\rho-\beta)}{\ell} n(t)+\sum_{i=1}^{6} \lambda_{i} C_{i}(t)  \tag{17.10}\\
\frac{\partial C_{i}(t)}{\partial t}=-\lambda_{i} C_{i}(t)+\frac{\beta_{i}}{\ell} n(t)
\end{array}\right.
$$

Expressed in this form, it should be borne in mind that $\ell$ integrates the $k_{\text {eff }}(t)$ (which is why it is called the effective lifetime of prompt neutrons or generation time). It must not be confused with the average lifetime of prompt and delayed neutrons, $\bar{\ell}$, which includes delayed neutrons with a lifetime 1000 -fold greater. These equations are considered by assuming that $\ell$ is almost constant, thereby implying a reasonable change in reactivity. Where this is not the case, it is better to use equations in which $\ell_{0}$ is explicitly utilized. The form of the point-kinetics equations allows a simple physical analysis of the neutron population. Nevertheless, the spatial effects should be carefully taken into account using an appropriate weight of the neutron parameters in the model (lifetime, delayed neutron fraction). If the equation on the precursor concentrations is summed on the number of precursor groups, the following is obtained:

$$
\sum_{i} \frac{\partial C_{i}(t)}{\partial t}=\sum_{i}-\lambda_{i} C_{i}(t)+\sum_{i} \frac{\beta_{i}}{\ell} n(t)-\sum_{i} \lambda_{i} C_{i}(t)+\frac{\beta}{\ell} n(t)
$$

Adding this equation to the first equation on $n(t)$ leads to:

$$
\frac{\partial\left[n(t)+\sum_{i} C_{i}(t)\right]}{\partial t}=\frac{\rho}{\ell} n(t)
$$

The sum of precursor concentrations $C_{\text {tot }} \equiv \sum_{i} C_{i}(t)$ is the amount of potential neutrons in the reactor. In general, this is more than the amount of neutrons actually present in the reactor. If reactivity $\rho$ is positive, the amount of neutrons $n(t)+C_{t o t}$ increases. If $\rho$ is negative, $n(t)+C_{\text {tot }}$ decreases. It should be noted that if $\rho$ is negative (respectively positive), $n(t)$ may increase (respectively decrease) if $C_{\text {tot }}$ decreases (respecively increases). This is contrary to the common belief that if $\rho$ is negative, $n(t)$ always decreases (respectively $\rho$ positive, $n(t)$ increases). However, this is true if the insertion of reactivity occurs during a permanent state in which $n(t)$ and $C_{\text {tot }}$ are constant. In a transient situation, the analysis should be done for each case (the history of the neutron population $n(t)$ and $C_{t o t}$ is required).

### 17.4.3 Mobile Fuel

The case in which the fuel is mobile, as for molten salt reactors or in experiments in which the fuel is oscillated (e.g. in the progressive poisoning method of Gérard Gambier), requires a transport term for precursors with velocity $V(t)$ along the $z$ axis:

$$
\frac{\partial C_{i}(\vec{r}, t)}{\partial t}+V(t) \frac{\partial C_{i}(\vec{r}, t)}{\partial z}=-\lambda_{i} C_{i}(\vec{r}, t)+\frac{\beta_{i}}{\ell} n(\vec{r}, t)
$$

### 17.5 Nordheim Equation

If the flux is factorized as the product of a spatial function and a time function (Glasstone and Edlund 1972, p. 297):

$$
\left\{\begin{array}{l}
\Phi(\vec{r}, t)=\Phi_{0}(\vec{r}) e^{\omega t} \\
C^{i}(\vec{r}, t)=C_{0}^{i}(\vec{r}) e^{\omega t}
\end{array}\right.
$$

it may be assumed that the reactor is close to the critical state, i.e. $\Phi_{0}(\vec{r})$ obeys the fundamental mode $\Delta \Phi_{0}(\vec{r})+B_{g}^{2} \Phi_{0}(\vec{r})=0$.
where: $\left(\omega+\lambda_{i}\right) C_{0}^{i}=\beta_{i} k_{\infty} \Sigma_{a} \Phi_{0}$
and: $\left[k_{e f f}(1-\beta)-1\right] \Phi_{0}+\sum_{i=1}^{6} \frac{\lambda_{i} C_{i 0}}{\Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)}=\ell_{B_{g}} \omega \Phi_{0}$
By substituting $C_{i 0}$ by its expression in terms of $\Phi_{0}$, removing the latter, and introducing the reactivity term, the previous equation is written as :

Nordheim Equation: $\quad \rho=\frac{k_{\text {eff }}-1}{k_{\text {eff }}}=\frac{\ell_{B_{g}} \omega}{1+\ell_{B_{g}} \omega}+\frac{1}{1+\ell_{B_{g}} \omega} \sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}$
This is the first form of the Nordheim Equation (after Lothar W. Nordheim), ${ }^{6}$ also known as the "Inhour Equation" (Hetrick 1993, p. 20; Ash 1979, p. 31). This equation has seven roots (for a standard 6-group delayed neutron calculation) called the frequencies. By definition, $k_{\text {eff }}$ tends to 1 where $\rho$ tends to infinity, and where $k_{\text {eff }}$ tends to zero (non-multiplying medium) $\rho$ tends to $-\infty$. This equation can be analyzed graphically giving the seven frequencies, i.e. the solutions to the Nordheim Equation for a given reactivity, by drawing a horizontal line with equation $\rho=f(\omega)$ in the diagram (Photo 17.2).

The points of intersection with the Nordheim curve give the solutions. In Fig. 17.10, the solutions for "positive reactivity" and "negative reactivity" are shown. In the latter case, it can be seen graphically that all roots are negative, indicating that the neutron population will decrease in an exponential manner, and at infinity, it will behave as the most negative root, i.e. the largest period of the reactor. Hence, for any anti-reactivity inserted, the convergence of the reactor cannot be faster than the radioactive decay of ${ }_{35}^{87} \mathrm{Br}$. However, in the case of a reactivity insertion, one root is always positive and can increase indefinitely when $\rho$ tends to 1 , i.e. $\rho$ is much larger than $\beta-$, which is synonymous for prompt critical behavior that leads to an explosion. Graphically, as reactivity approaches $\beta$, the effect of a shorter generation time tends to increase the frequency $\omega_{1}$, thereby leading to a much faster increase in the neutron population in the event of reactivity insertion. The second form of the Nordheim Equation is obtained by setting $\ell=\ell_{B_{g}} / k_{\text {eff }}$. From the first form, the following may be written:

[^343]

Photo 17.2 Lothar Nordheim in 1954 (Duke University)


Fig. 17.10 Graphical representation of the first form of the Nordheim Equation

$$
\rho\left(1+\ell_{B_{g}} \omega\right)=\ell_{B_{g}} \omega+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}
$$

where

$$
\rho=-\ell_{B_{g}} \omega(\rho-1)+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}=-\ell_{B_{g}} \omega\left(\frac{k_{e f f}-1}{k_{e f f}}-1\right)+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}=
$$

$\frac{\ell_{B_{g}}}{k_{\text {eff }}} \omega+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}$
Thus:

Second form of the Nordheim Equation: $\quad \rho=\ell \omega+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}$
It should be pointed out that for large values of $\omega$, the function $\rho=\ell \omega+\sum_{i=1}^{6}$ $\beta_{i} \omega /\left(\omega+\lambda_{i}\right)$ tends to $\rho=\ell \omega+\beta$. Yet, by definition, $\rho$ cannot increase beyond 1. The introduction of $\ell=\ell_{B_{g}} / k_{\text {eff }}$, which is not constant since it depends on $\rho$ via the formula $k_{\text {eff }}=1 /(1-\rho)$, shows that the graph of $\rho=\ell \omega+\beta$ is not a straight line, as is often shown in several reference books. This is the case for small reactivity changes under the hypothesis that $\ell \approx$ constant (Fig. 17.11).

The roots $\omega_{i}$ are once again the abscissa of the intersection of the plot $\omega=f(\rho)$ with the horizontal line of abscissa $\rho$. The ordinate gives the reactivity (and not $\rho / \beta$ as in Fig. 17.10), the region with $\rho>1$ is not possible by definition of reactivity. Several references [including Hetrick (1993)] present the graphic solution in the previous manner, with the axes inverted as in Fig. 17.12. The Nordheim Equation may also be established by direct formulation. Where $n(t)$ is the number of neutrons emitted in a generation and $\ell_{B_{g}}$ the lifetime in finite medium during $\Delta t, n(t) \Delta t / \ell_{B_{g}}$ neutrons are lost and they create $k_{\text {eff }}(1-\beta) n(t) \Delta t / \ell_{B_{g}}$ prompt neutrons and $\Sigma_{i} \lambda_{i} C_{i}$ delayed neutrons.

$$
\left\{\begin{array}{l}
\frac{d n(t)}{d t}=k_{e f f}(1-\beta) \frac{n(t)}{\ell_{B_{g}}}-\frac{n(t)}{\ell_{B_{g}}}+\sum_{i=1}^{6} \lambda_{i} C_{i} \\
\frac{d C_{i}}{d t}=k_{e f f} \beta_{i} \frac{n(t)}{\ell_{B_{g}}}-\lambda_{i} C_{i}
\end{array}\right.
$$



Fig. 17.11 Graphical representation of the second form of the Nordheim Equation


Fig. 17.12 Graphical representation of the second form of the Nordheim Equation Graphical plot of the form $\omega=g(\rho)$

Since: $\beta_{i} k_{\infty} \Sigma_{a} \Phi=\beta_{i} k_{\infty} \underbrace{\Sigma_{a} v}_{\frac{1}{\tau_{0}}} n(t)=\beta_{i} \frac{k_{\infty}}{\ell_{0}} n(t)$ and: $\frac{k_{\infty}}{\ell_{0}}=\frac{k_{\text {eff }}}{\ell_{B_{g}}}$
the previous formulation is obtained. Finally, the neutron population and the precursor concentrations are the sum of the seven exponential terms (in a six-delayed-neutron-group calculation), or more generally, of the $n_{r}+1$ exponential terms if $n_{r}$ is the number of delayed neutron groups.

$$
n(t)=\sum_{k=1}^{7} A_{k} e^{\omega_{k} t} \quad C_{i}(t)=\sum_{k=1}^{7} \gamma_{i k} e^{\omega_{k} t}
$$

The divergence period $T$ is the time such that $n(t)$ is multiplied by the Neper constant $e$ in the reactor (or stable period). When $t$ increases, the positive solution $\omega_{1}$ gives asymptotic behavior (if $\rho>0$ ):

$$
n(t) \approx A_{1} e^{\omega_{1} t}
$$

The divergence period in this case is worth $T=1 / \omega_{1}$. If $\rho<0, \omega_{1}$ is the less negative root. Then, $n(t) \approx A_{1} \quad e^{\omega_{1} t}$, and $T=\left|\omega_{1}\right|^{-1}$. If $\rho \ll 1$, then $\ell_{B_{g}} \omega \approx \ell \omega \ll 1$ :

$$
\rho \approx \ell \omega+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\lambda_{i}} \Rightarrow \omega=\frac{\ell}{\ell+\sum_{i=1}^{6} \beta_{i} / \lambda_{i}}
$$

If $\rho$ tends to 1 , the divergence period tends to 0 , i.e. the reactor can be made to diverge as fast as desired. If $\rho$ tends to $-\infty$, the divergence period tends to $1 / \lambda_{1}$, i.e. the mean lifetime of the precursor having the longest period $(\sim 57 \mathrm{~s})$. This limits overwhelming of the chain reaction by natural decay. Taking $T=1 / \omega_{1}, \rho$ can be tied to the divergence period as:

Hence: $\quad \rho=\frac{k_{\text {eff }}-1}{k_{\text {eff }}}=\frac{\ell \omega}{1+\ell \omega}+\frac{1}{1+\ell \omega} \sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}$
If $\ell \omega$ is diregarded compared to 1 , which is acceptable, the reactivity equation can be simplified:

$$
\rho \approx \ell \omega+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}=\frac{\ell}{T}+\sum_{i=1}^{6} \frac{\beta_{i}}{1+\lambda_{i} T}
$$

This form of the Nordheim Equation led to it being called the "Inhour Equation" (the period being the inverse of time). 1 Inhour is the amount of positive reactivity corresponding to an asymptotic increase of power for a reactor period of 1 h . In the English-speaking world, the "Dollar" unit (symbol $\$$ ) is obtained by dividing the reactivity $\rho$ by $\beta$. Therefore, a reactivity of 2 Dollars is obtained if $\rho=2 \beta$.

## 17.6 "Prompt Jump" Notion: Insertion of a Reactivity Step

Assuming that the reactor is initially in a critical state at equilibrium, an "instantaneous" amount of reactivity is inserted by some means (e.g. boron dilution with an amount of non-borated or insufficiently-borated water, rod removal, etc.) (Fig. 17.13).

For $\mathrm{t}<0, \frac{\partial C_{i}}{\partial t}=0 \Rightarrow C_{i}^{0}=\frac{\beta_{i}}{\lambda_{i}}\left(k_{\infty} \Sigma_{a}\right)_{0^{-}} \Phi_{0}$

Fig. 17.13 Insertion of a reactivity step


For $t=0$, the flux and precursor concentrations are continuous. The flux is given with six delayed-neutron groups, and the precursor concentration by:

$$
\Phi=\Phi_{0} \sum_{k=1}^{7} \alpha_{k} e^{\omega_{k} t} \text { and } C_{i}=C_{i}^{0} \sum_{k=1}^{7} \gamma_{i k} e^{\omega_{k} t}
$$

For $t>0$, the following is obtained:

$$
\frac{\partial C_{i}}{\partial t}=C_{i}^{0} \sum_{k=1}^{7} \omega_{k} \gamma_{i k} e^{\omega_{k} t}=\beta_{i}\left(k_{\infty} \Sigma_{a}\right)_{0^{+}} \Phi_{0} \sum_{k=1}^{7} \alpha_{k} e^{\omega_{k} t}-\lambda_{i} C_{i}^{0} \sum_{k=1}^{7} \gamma_{i k} e^{\omega_{k} t}
$$

where: $\quad C_{i}^{0} \gamma_{i k}=\beta_{i}\left(k_{\infty} \Sigma_{a}\right)_{0^{+}} \Phi_{0} \frac{\alpha_{k}}{\omega_{k}+\lambda_{i}} \quad$ for $\left\{\begin{array}{l}i=1 \text { to } 6 \\ k=1 \text { to } 7\end{array}\right.$
Thus: $C_{i}^{0}=\sum_{k=1}^{7} C_{i}^{0} \gamma_{i, k}=\beta_{i}\left(k_{\infty} \Sigma_{a}\right)_{0^{+}} \Phi_{0} \sum_{k=1}^{7} \frac{\alpha_{k}}{\omega_{k}+\lambda_{i}}=\frac{\beta_{i}}{\lambda_{i}}\left(k_{\infty} \Sigma_{a}\right)_{0^{-}} \Phi_{0}$
The sum of the previous equation can also be computed:

$$
\begin{aligned}
& \sum_{k=1}^{7} \frac{\alpha_{k}}{\omega_{k}+\lambda_{i}}=\frac{\left(k_{\infty} \Sigma_{a}\right)_{0^{-}}}{\left(k_{\infty} \Sigma_{a}\right)_{0^{+}}} \frac{1}{\lambda_{i}} i=1 \text { to } 6 \\
& \quad \text { and } \sum_{k=1}^{7} \alpha_{k}=1
\end{aligned}
$$

After a sufficiently long time, the flux behaves as a growing exponential term: $\Phi \approx \Phi_{0} \alpha_{1} e^{\omega_{1} t}$ since the only root is positive. For short times, the effect due to the other exponential terms fades out quickly, such that the flux increases very rapidly to take the shape of a jump, known as a "prompt jump" (Lamarsh and Baratta 2001, p. 343; Weaver 1968, p. 49) (Fig. 17.14).

Fig. 17.14 Behavior of flux after insertion of a reactivity step $\rho>0$ at time $\mathrm{t}=0$


### 17.7 Age Theory in the Kinetics Equation for Thermal Neutrons

(Meghreblian and Holmes 1960, p. 551)
The neutron kinetics equation for one energy group was established earlier. However, the neutron diffusion equation can be corrected to account for thermal neutrons by determining the non-leakage factor $e^{-B_{g}^{2} \tau_{t h}}$ during slowing-down in the Fermi age theory, with $B_{g}^{2}$ being the geometrical buckling of the pile. Let the thermal neutron diffusion equation be:
$D \Delta \Phi_{t h}-\Sigma_{a} \Phi_{t h}+S=\frac{1}{v} \frac{\partial \Phi_{t h}}{\partial t}$ where $\Phi_{t h}$ is the thermal flux.
Neglecting the start-up sources, the thermal neutron source term can be written as:
$S=k_{\infty} \Sigma_{a} \Phi_{t h} e^{-B_{g}^{2} \tau_{t h}}$ in thermal neutrons per $\mathrm{cm}^{3}$ and per second
The source term originates from fast neutrons, i.e. $k_{\infty} \Sigma_{a} \Phi_{t h} / p$. These fast neutrons can either be captured during the slowing-down process, leaving $p \times k_{\infty} \Sigma_{a} \Phi_{t h} / p$ neutrons, or else they can escape the pile with a non-leakage probability of $e^{-B_{g}^{2} \tau_{l h}}$, leaving $k_{\infty} \Sigma_{a} \Phi_{t h} e^{-B_{g}^{2} \tau_{l h}}$ neutrons (Fig. 17.15).

Accounting for delayed neutrons divides the neutron source term into two parts: a source of prompt fast neutrons, $(1-\beta) k_{\infty} \Sigma_{a} \Phi_{t h} / p$, and a source of delayed fast neutrons, $\sum_{i} \beta_{i} k_{\infty} \Sigma_{a} \Phi_{t h} / p=\sum_{i} \lambda_{i} C_{i}$. The thermal neutrons corresponding to these two fast neutron sources are obtained by multiplying by the non-leakage probability $e^{-B_{g}^{2} \tau_{l h}}$ and by the resonance escape probability $p$, to give the thermal neutron source:


Fig. 17.15 Blaquière representation of kinetics equation of thermal neutrons

$$
S_{t h}=(1-\beta) k_{\infty} \Sigma_{a} \Phi_{t h} e^{-B_{g}^{2} \tau_{t h}}+\left(\sum_{i} \lambda_{i} C_{i}\right) p e^{-B_{g}^{2} \tau_{t h}}
$$

Hence $: \frac{1}{v} \frac{\partial \Phi_{t h}}{\partial t}=D \Delta \Phi_{t h}-\Sigma_{a} \Phi_{t h}+(1-\beta) k_{\infty} \Sigma_{a} \Phi_{t h} e^{-B_{g}^{2} \tau_{l h}}+\left(\sum_{i} \lambda_{i} C_{i}\right) p e^{-B_{g}^{2} \tau_{t h}}$
Introducing the thermal scattering area, $L^{2} \equiv D / \Sigma_{a}$, and the lifetime of prompt ${ }^{7}$ neutrons in an infinite medium, $\ell_{0} \equiv 1 /\left(v \Sigma_{a}\right)$, the following is obtained (Fig. 17.16):

$$
\begin{aligned}
\ell_{0} \frac{\partial \Phi_{t h}}{\partial t}= & L^{2} \Delta \Phi_{t h}+\left((1-\beta) k_{\infty} e^{-B_{g}^{2} \tau_{t h}}-1\right) \Phi_{t h} \\
& +p \frac{e^{-B_{g}^{2} \tau_{t h}}}{\Sigma_{a}}\left(\sum_{i} \lambda_{i} C_{i}\right)
\end{aligned}
$$

This equation is identical to that obtained in the chapter on neutron diffusion using the "large-size reactor" approximation:

$$
e^{-B_{g}^{2} \tau_{t h}} \approx 1-B_{g}^{2} \tau_{t h} \text { and } M^{2}=L^{2}+\tau_{t h}
$$

The precursor equation is given by:

$$
\frac{\partial C_{i}}{\partial t}=-\lambda_{i} C_{i}+\beta_{i} \frac{k_{\infty}}{p} \Sigma_{a} \Phi
$$

Similar to the space-time decomposition of the flux and the precursor concentrations as seen previously, the following is set:

$$
\left\{\begin{array}{l}
\Phi_{t h}(\vec{r}, t)=\Phi_{0}(\vec{r}) e^{\omega t} \\
C_{i}(\vec{r}, t)=C_{i 0}(\vec{r}) e^{\omega t}
\end{array}\right.
$$

and, assuming that the reactor is close to a critical state, the flux obeys a fundamental mode:

$$
\Delta \Phi_{0}(\vec{r})+B_{g}^{2} \Phi_{0}(\vec{r})=0
$$

where: $C_{i, 0}(\vec{r}) \omega e^{\omega t}=-\lambda_{i} C_{i} e^{\omega t}+\frac{k_{\infty}}{p} \beta_{i} \Sigma_{a} \Phi_{0}(\vec{r}) e^{\omega t}$

[^344]

Fig. 17.16 Delayed neutrons (six groups) in the Blaquière representation
thus:

$$
C_{i, 0}(\vec{r})=\frac{k_{\infty}}{p} \frac{\beta_{i}}{\left(\omega+\lambda_{i}\right)} \Sigma_{a} \Phi_{0}(\vec{r})
$$

This formula leads to computation of the initial precursor concentrations. Inserting this expression in the neutron kinetics equation, the following is obtained:

$$
\begin{array}{r}
\ell_{0} \Phi_{0}(\vec{r}) \omega e^{\omega t}=-L^{2} e^{\omega t} B_{g}^{2} \Phi_{0}(\vec{r})+\left[(1-\beta) k_{\infty} e^{-B_{8}^{2} \tau_{l \mid}}-1\right] \Phi_{0}(\vec{r}) e^{\omega t} \\
+p \frac{e^{-B_{8}^{2} \tau_{t h}}}{\Sigma_{a}}(\sum_{i} \lambda_{i} e^{\omega t} \underbrace{\frac{k_{\infty}}{p} \frac{\beta_{i}}{\left(\omega+\lambda_{i}\right)} \Sigma_{a} \Phi_{0}(\vec{r})}_{c_{i, 0}(\vec{r})})
\end{array}
$$

Which, by eliminating $\Phi_{0}(\vec{r}) e^{\omega t}$, can be simplified to:

$$
\ell_{0} \omega=-L^{2} B_{g}^{2}-1+(1-\beta) k_{\infty} e^{-B_{g}^{2} \tau_{l h}}+k_{\infty} e^{-B_{g}^{2} \tau_{l h}} \sum_{i} \frac{\lambda_{i} \beta_{i}}{\omega+\lambda_{i}}
$$

Using the neutron lifetime in the geometry with buckling $B_{g}$ : $\ell_{B_{g}}=\ell_{0} /\left(1+L^{2} B_{g}^{2}\right)$, then: $k_{\text {eff }}=k_{\infty} e^{-B_{g}^{2} \tau_{t / t}} /\left(1+L^{2} B_{g}^{2}\right)$, and using the proportion of the delayed neutrons $\beta=\sum_{i} \beta_{i}$, the following equation is reached:

$$
k_{e f f}-1=\ell_{B_{g}} \omega+k_{\text {eff }} \sum_{i} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}
$$

Inserting the reactivity $\rho \equiv\left(k_{\text {eff }}-1\right) / k_{\text {eff }}$, the classical Nordheim Equation is established:

$$
\rho=\frac{\ell_{B_{g}} \omega}{1+\ell_{B_{g}} \omega}+\frac{1}{1+\ell_{B_{g}} \omega} \sum_{i} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}
$$

### 17.8 Reduced Kinetics Equations

Let the differential equations for neutron kinetics previously encountered be:

$$
\left\{\begin{array}{c}
\frac{d n(t)}{d t}=k_{e f f}(1-\beta) \frac{n(t)}{\ell_{B_{g}}}-\frac{n(t)}{\ell_{B_{g}}}+\sum_{i=1}^{6} \lambda_{i} C_{i}(t) \\
\frac{d C_{i}(t)}{d t}=\frac{k_{e f f} \beta_{i}}{\ell_{B_{g}}} n(t)-\lambda_{i} C_{i}(t)
\end{array}\right.
$$

The second form of the Nordheim equation is obtained by setting $\ell \equiv \ell_{B_{g}} / k_{e f f}=\ell_{B_{g}}(1-\rho)$. In general, it is assumed that $\ell$ varies weakly.

$$
\left\{\begin{array}{c}
\frac{d n(t)}{d t}=\frac{\rho-\beta}{\ell} n(t)+\sum_{i=1}^{6} \lambda_{i} C_{i}(t) \\
\frac{d C_{i}(t)}{d t}=\frac{\beta_{i}}{\ell} n(t)-\lambda_{i} C_{i}(t)
\end{array}\right.
$$

Several works use the reduced equation above only, which can lead to confusion regarding the value of $\ell$, about which the reader should take care. Henceforth, the term $\ell$ will be used as far as possible. ${ }^{8}$ In the chapter dedicated to fission, data is given concerning the six delayed neutron groups.

The data on the six delayed neutron groups were presented in the chapter on fission. The value of $\lambda$, denoting an average delayed neutron group, is obtained as follows:

$$
\lambda=\frac{\beta}{\sum_{i=1}^{6} \beta_{i} / \lambda_{i}} .
$$

If all precursors are properly known, this formula may be generalized as follows:

$$
\lambda=\frac{\beta}{\sum_{\text {precursors }} \beta_{i} / \lambda_{i}}
$$

The following table gives the classical values for the main fissile systems (Tables 17.5 and 17.6):

[^345]|  |  | Keepin <br> $(1965$, <br> p. 166) | Hetrick <br> $(1993$, <br> p. 6) | Ott and <br> Neuhold <br> $(1985, ~ p .24)$ | Reuss <br> $(2003$, <br> p. 119) |
| :--- | :--- | :--- | :--- | :--- | :--- |
| Prompt neutron lifetime <br> in an infinite medium | $\ell_{0}=\frac{1}{\mathrm{v} \Sigma_{a}}$ |  | $\ell_{\infty}$ | $\ell_{\infty}$ |  |
| Prompt neutron lifetime <br> in a finite medium | $\ell_{B_{g}}=\frac{\ell_{0}}{1+L^{2} B_{g}^{2}}$ | $\ell$ | $\ell_{0}$ | $\ell$ | $\theta$ |
| Effective prompt neutron <br> lifetime or generation <br> time | $\ell=\frac{\ell_{B_{g}}}{k_{\text {eff }}}=\frac{1}{v \nu \Sigma_{f}}$ | $\Lambda$ | $\ell$ | $\Lambda$ | $\ell$ |

Table 17.5 Kinetic data for thermal fission

| Isotope | $\nu$ | $\beta$ | $\beta / \lambda$ | $\lambda$ |
| :--- | :--- | :--- | :--- | :--- |
| ${ }^{233} U$ | 2.2866 | 0.00281 | 0.050 s | $0.0562 \mathrm{~s}^{-1}$ |
| ${ }^{235} U$ | 2.2423 | 0.00700 | 0.089 s | $0.0787 \mathrm{~s}^{-1}$ |
| ${ }^{239} \mathrm{Pu}$ | 2.8799 | 0.00227 | 0.033 s | $0.0688 \mathrm{~s}^{-1}$ |
| ${ }^{241} \mathrm{Pu}$ | 2.9340 | 0.00545 | 0.060 s | $0.0908 \mathrm{~s}^{-1}$ |

Table 17.6 Kinetic data for fast fission (based on $U_{235}$ spectrum)

| Isotope | $\nu$ | $\beta$ | $\beta / \lambda$ | $\lambda$ |
| :--- | :--- | :--- | :--- | :--- |
| ${ }^{232} \mathrm{Th}$ | 2.44 | 0.02230 | 0.225 s | $0.0991 \mathrm{~s}^{-1}$ |
| ${ }^{233} \mathrm{U}$ | 2.62 | 0.00266 | 0.048 s | $0.0665 \mathrm{~s}^{-1}$ |
| ${ }^{235} U$ | 2.57 | 0.00660 | 0.084 s | $0.0786 \mathrm{~s}^{-1}$ |
| ${ }^{238} \mathrm{U}$ | 2.79 | 0.01610 | 0.124 s | $0.1300 \mathrm{~s}^{-1}$ |
| ${ }^{239} \mathrm{Pu}$ | 3.09 | 0.00212 | 0.031 s | $0.0684 \mathrm{~s}^{-1}$ |
| ${ }^{240} \mathrm{Pu}$ | 3.32 | 0.00289 | 0.038 s | $0.0743 \mathrm{~s}^{-1}$ |
| ${ }^{241} \mathrm{Pu}$ | 2.99 | 0.00544 | 0.062 s | $0.0877 \mathrm{~s}^{-1}$ |

From Keepin and Lewins, referenced by R. Barjon

It is clear that if $\beta$ varies significantly according to the fissile or fertile isotope in question, from 0.0223 for ${ }^{232} \mathrm{Th}$ to 0.00227 for ${ }^{239} \mathrm{Pu}$ (i.e. tenfold), the value of $\lambda$, perhaps more important for kinetics, remains around 0.08 , corresponding to a mean lifetime for precursors of 12.5 s .

### 17.9 Kinetics with an Imposed Neutron Source

The particular case of a neutron source independent of the flux, such as the spontaneous fission of some heavy nuclei or an external neutron source as for Accelerator Driven Systems (ADS, in which a particle accelerator powers a subcritical reactor by firing a beam at a neutron-producing target), may be approached with the Laplace transform. Let the kinetics equation with a source be:

$$
\left\{\begin{array}{c}
\frac{d n(t)}{d t}=\frac{\rho-\beta}{\ell} n(t)+\sum_{i=1}^{6} \lambda_{i} C_{i}(t)+q(t) \\
\frac{d C_{i}(t)}{d t}=\frac{\beta_{i}}{\ell} n(t)-\lambda_{i} C_{i}(t)
\end{array}\right.
$$

With $\mathrm{n}(p), \mathrm{C}_{\mathrm{i}}(p)$ and $\mathrm{q}(p)$ the Laplace transforms of the time variable of $n(t)$, $C_{i}(t)$ and $q(t)$, the following is obtained (Weaver 1963, p. 40):

$$
\left\{\begin{array}{c}
p \mathrm{n}(p)-n(0)=\frac{\rho-\beta}{\ell} \mathrm{n}(p)+\sum_{i=1}^{6} \lambda_{i} \mathrm{C}_{\mathrm{i}}(p)+\mathrm{q}(p) \\
p \mathrm{C}_{\mathrm{i}}(p)-C_{i}(0)=\frac{\beta_{i}}{\ell} \mathrm{n}(p)-\lambda_{i} \mathrm{C}_{\mathrm{i}}(p)
\end{array}\right.
$$

Using a mathematical shortcut in which $\mathrm{n}(p)$ is set as the product $\mathrm{K}(p) \mathrm{N}(p)$, which is invertible by an inverse Laplace transform, and where $\mathrm{N}(p)$ is the image of the solution without an imposed source:

$$
\left\{\begin{array}{c}
\mathrm{K}(p)=n(0)+q(p)+\sum_{i=1}^{6} \frac{\lambda_{i} C_{i}(0)}{\lambda_{i}+p} \\
\mathrm{~N}(p)=\frac{\ell}{\ell p-\rho+p \sum_{i=1}^{6} \frac{\beta_{i}}{\lambda_{i}+p}}
\end{array}\right.
$$

For a constant source, $q(t)=Q$, the inverse Laplace leads to:

$$
\left\{\begin{array}{l}
n(t)=\sum_{i=0}^{6} \frac{\alpha_{i}}{\omega_{i}}\left(\left(e^{\omega_{i} t}-1\right) Q+e^{\omega_{i} t} \frac{\rho n(0)}{\ell}\right) \\
\rho=\ell \omega_{i}+\sum_{i=1}^{6} \frac{\beta_{i} \omega_{i}}{\lambda_{i}+\omega_{i}} \quad \text { pour } \omega_{i}=0 \text { à } 6
\end{array}\right.
$$

The values of $\omega_{i}$ are the roots of the second form of the Nordheim equation. For a critical pattern ( $\rho=0$ where $\omega_{0}=0$ ), the following is obtained (Fig. 17.17):

$$
n(t)=n(0)+\alpha_{0} Q t+\sum_{i=1}^{6} \frac{\alpha_{i}}{\omega_{i}}\left(\left(e^{\omega_{i} t}-1\right) Q+e^{\omega_{i} t} \frac{\rho n(0)}{\ell}\right)
$$

Wyman and Harms generalized this approach ${ }^{9}$ by projecting the flux onto a basis of fundamental modes from a two-group diffusion equation and one group of delayed neutrons.

### 17.10 Delayed Neutron Spectrum

The delayed neutron spectrum, often noted as $\chi_{d}(E)$ (the index $p$ denotes prompt neutrons) or $\chi_{1}(E)$ (the index 0 here denotes prompt neutrons), is not identical to the prompt neutron emission spectrum. The two deviate, especially at low energies. On

[^346]

Fig. 17.17 Evolution of reactor with imposed source
average, the energy of delayed neutrons is of the order of 400 keV rather than the 2 MeV mean energy of the prompt neutrons. The spectrum of delayed neutrons released by the main emitters was measured very precisely by Greenwood and Watts. ${ }^{10}$ In the continuous-energy model with one group of delayed neutrons, the neutrons are counted whatever their energy. This approximation may be corrected by introducing the effective beta, $\beta_{\text {eff }}$, obtained by weighting $\beta$ by the adjoint fluxes or importances of the two intensities of the prompt and delayed neutrons using a formalism set up by G. Keepin ${ }^{11}$ (1965, p. 164) (Fig. 17.18).

These importances, with a weight of 0.97 in $P W R$, suggest that $\beta_{\text {eff }}$ is smaller than $\beta$. The importance function (the adjoint flux with the fission source as adjoint source) $\Phi^{*}(\vec{r}, E)$ is the probability of a neutron at position $\vec{r}$ and energy $E$ inducing fission somewhere inside the reactor (Stacey 2001, p. 141). The relative importance of the delayed neutrons of group $I$ of the fissile isotope $F$ is given by ${ }^{12,13}$ :

[^347]

Fig. 17.18 Emission spectra by group of delayed neutrons (adapted from Batchelor and Hyder) analyzed by Keepin (1965, p. 94) and Weaver (1964, p. 340)

$$
I_{d, i}^{F}=\int_{V} d \vec{r} \int_{E=0}^{\infty} \chi_{d, i}^{F}(E) \Phi^{*}(\vec{r}, E) d E \int_{E^{\prime}=0}^{\infty} \nu \Sigma_{f}^{F} \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}
$$

The importance of the prompt neutrons is given by:

$$
I_{p}^{F}=\int_{V} d \vec{r} \int_{E=0}^{\infty} \chi_{p}^{F}(E) \Phi^{*}(\vec{r}, E) d E \int_{E^{\prime}=0}^{\infty} \nu \Sigma_{\text {fission }}^{F} \Phi\left(\vec{r}, E^{\prime}\right) d E^{\prime}
$$

These importances enable the calculation of an importance function used to transform the delayed neutron fraction to the effective fraction used in a pointkinetics model (Fig. 17.19):

$$
\beta_{i, e f f}^{F}=\frac{I_{d, i}^{F} \beta_{i}^{F}}{\sum_{F}\left[\left(1-\sum_{i} \beta_{i}^{F}\right) I_{p}^{F}+\sum_{i} I_{d, i}^{F} \beta_{i}^{F}\right]}
$$

The delayed neutron spectrum is integrated for multi-group kinetics equations. Let $G$ be the number of energy groups with six groups of delayed neutrons (in the standard model):


Fig. 17.19 Total emission spectrum for delayed neutrons (adapted from Batchelor and Bonner) analyzed by Keepin (1965, p. 93)

$$
\left\{\begin{array}{cc}
\frac{\frac{1}{v_{g}} \frac{\partial \Phi_{g}}{\partial t}=D_{g} \Delta \Phi_{g}-\Sigma_{a g} \Phi_{g}+\sum_{g^{\prime}=1}^{G} \Sigma_{g^{\prime} \rightarrow g} \Phi_{g^{\prime}}+(1-\beta) \chi_{0, g}\left(\sum_{g^{\prime}=1}^{G} \nu \Sigma_{f_{g}} \Phi_{g}\right)+\sum_{i=1}^{6} \chi_{i, g} \lambda_{i} C_{i}}{\frac{\partial C_{i}}{\partial t}=\beta_{i}\left(\sum_{g^{\prime}=1}^{6} \nu \Sigma_{f_{g}} \Phi_{g}\right)-\lambda_{i} C_{i}} & g=1, G \\
& i=1,6
\end{array}\right.
$$

$\chi_{0, g}$ is the prompt neutron spectrum and $\chi_{1, g}$ is the normalized spectrum of delayed neutrons, both normalized such that:

$$
\sum_{g=1}^{G} \chi_{0, g}=1 \text { and } \sum_{g=1}^{G} \chi_{1, g}=1
$$

for $i=1,6$. The $P W R$ are often calculated with two energy groups (thermal cut-off at 0.625 eV$)$. Thus:

$$
\left\{\begin{array}{c}
\frac{1}{v_{1}} \frac{\partial \Phi_{1}}{\partial t}=D_{1} \Delta \Phi_{1}-\left(\Sigma_{a_{1}}+\Sigma_{r}\right) \Phi_{1}+(1-\beta) \chi_{0}\left(\nu \Sigma_{f_{1}} \Phi_{1}+\nu \Sigma_{f_{2}} \Phi_{2}\right)+\sum_{i=1}^{6} \chi_{i, 1} \lambda_{i} C_{i} \\
\frac{1}{v_{2}} \frac{\partial \Phi_{2}}{\partial t}=D_{2} \Delta \Phi_{2}-\Sigma_{a_{2}} \Phi_{2}+\Sigma_{r} \Phi_{1} \\
\frac{\partial C_{i}}{\partial t}=\beta_{i}\left(\nu \Sigma_{f_{1}} \Phi_{1}+\nu \Sigma_{f_{2}} \Phi_{2}\right)-\lambda_{i} C_{i}
\end{array}\right.
$$

It has been assumed that no neutrons are created in thermal group 2 other than by scattering ( $\Sigma_{r} \Phi_{1}$ with $\Sigma_{r}=\Sigma_{1 \rightarrow 2}$ ) from group 1 ; while not rigorously accurate, this is acceptable for first-order effects. For a 3D reactor, the kinetic quantities must be spatially weighted. Writing the diffusion equation in matrix form, the following operators are used:

$$
\left\{\begin{aligned}
P & =\left[\begin{array}{cc}
\nu \Sigma_{f_{1}} & \nu \Sigma_{f_{2}} \\
0 & 0
\end{array}\right] \text { the production operator } \\
K & =\left[\begin{array}{cc}
\Sigma_{a_{1}}+\Sigma_{r}-D_{1} \Delta & 0 \\
-\Sigma_{r} & \Sigma_{a_{2}}-D_{2} \Delta
\end{array}\right] \text { where } \Delta \text { is the Laplace operator } \\
\Phi & =\left[\begin{array}{l}
\Phi_{1} \\
\Phi_{2}
\end{array}\right]
\end{aligned}\right.
$$

In the static case, the diffusion equation is written as: $\left(\frac{1}{k_{e f f}} P-K\right) \Phi=0$
Let the adjoint flux be $\Phi^{*}=\left[\Phi_{1}^{*}, \Phi_{2}^{*}\right]$, which verifies the adjoint system of equations:

$$
\Phi^{*}\left(\frac{1}{k_{e f f}} P^{*}-K^{*}\right)=0
$$

where the adjoint operators are the transpose of the direct operators (if all their terms are real):

$$
P^{*}=\left[\begin{array}{ll}
\nu \Sigma_{f_{1}} & 0 \\
\nu \Sigma_{f_{2}} & 0
\end{array}\right] \quad K^{*}=\left[\begin{array}{cc}
\Sigma_{a_{1}}+\Sigma_{r}-D_{1} \Delta & -\Sigma_{r} \\
0 & \Sigma_{a_{2}}-D_{2} \Delta
\end{array}\right]
$$

First-order perturbation theory gives the calculation of the change in reactivity $d \rho=-d\left(1 / k_{e f f}\right)$ with $\rho=1-\left(1 / k_{e f f}\right)$ :

$$
d \rho=\frac{\Phi^{*} \times\left(\frac{1}{k_{e f f}} d P-d K\right) \Phi}{\Phi^{*} \times P \Phi}
$$

where $\times$ is the matrix product with:

$$
\begin{aligned}
\Phi^{*} \times P \Phi & =\left[\Phi_{1}^{*}, \Phi_{2}^{*}\right]\left[\begin{array}{cc}
\nu \Sigma_{f_{1}} & \nu \Sigma_{f_{2}} \\
0 & 0
\end{array}\right]\left[\begin{array}{l}
\Phi_{1} \\
\Phi_{2}
\end{array}\right]=\left[\Phi_{1}^{*}, \Phi_{2}^{*}\right]\left[\begin{array}{c}
\nu \Sigma_{f_{1}} \Phi_{1}+\nu \Sigma_{f_{2}} \Phi_{2} \\
0
\end{array}\right] \\
& =\Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f_{2}} \Phi_{2}
\end{aligned}
$$

The thermal adjoint flux $\Phi_{2}^{*}$ no longer appears in the previous result, which is contrary to the (wrong) expression that would "naturally" be written:
$\Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1}+\Phi_{2}^{*} \nu \Sigma_{f_{2}} \Phi_{2}$. The matrix form of the kinetics equation may be expressed as:

$$
\begin{aligned}
& \left\{\begin{array}{l}
\frac{1}{v} \frac{\partial \Phi}{\partial t}=(1-\beta) P \Phi-K \Phi+\sum_{i=1}^{6} \lambda_{i} C_{i} \chi \\
\text { with } \frac{1}{v} \\
\frac{\partial \Phi}{\partial t}=\left[\begin{array}{cc}
\frac{1}{v_{1}} & \frac{\partial \Phi_{1}}{\partial t} \\
\frac{1}{v_{2}} & \frac{\partial \Phi_{2}}{\partial t}
\end{array}\right] \quad \text { and } \sum_{i=1}^{6} \lambda_{i} C_{i} \chi=\left[\begin{array}{c}
\sum_{i=1}^{6} \lambda_{i} C_{i} \chi_{i, 1} \\
0
\end{array}\right] \\
\frac{\partial C_{i}}{\partial t}=\beta_{i} \nu \Sigma_{f} \Phi-\lambda_{i} C_{i} \text { and } \nu \Sigma_{f} \Phi=\left[\nu \Sigma_{f_{1}}, \nu \Sigma_{f_{2}}\right]\left[\begin{array}{l}
\Phi_{1} \\
\Phi_{2}
\end{array}\right]=\nu \Sigma_{f_{1}} \Phi_{1}+\nu \Sigma_{f_{2}} \Phi_{2}
\end{array}\right.
\end{aligned}
$$

Classically, the solution is sought in the form of:

$$
\Phi=\left[\begin{array}{c}
\Phi_{1} \\
\Phi_{2}
\end{array}\right]=\alpha e^{\omega t}=\left[\begin{array}{cc}
\alpha_{1} & e^{\omega t} \\
\alpha_{2} & e^{\omega t}
\end{array}\right] \text { where: } \frac{\partial \Phi}{\partial t}=\omega \Phi \text { and, similarly: } \frac{\partial C_{i}}{\partial t}=\omega C_{i}
$$

with: $\omega C_{i}=\beta_{i} \nu \Sigma_{f} \Phi-\lambda_{i} C_{i}$

$$
\text { i.e.: } C_{i}=\frac{\beta_{i} \nu \Sigma_{f} \Phi}{\omega+\lambda_{i}}
$$

Hence: $\sum_{i=1}^{6} \lambda_{i} C_{i}=\sum_{i=1}^{6} \frac{\beta_{i} \lambda_{i}}{\omega+\lambda_{i}} \nu \Sigma_{f} \Phi$
Inserting the time derivative of the flux in the matrix form of the kinetics equation leads to:

$$
\left\{\begin{array}{l}
\omega \frac{1}{v} \Phi=(P-K) \Phi-\beta P \Phi+\sum_{i=1}^{6} \lambda_{i} C_{i} \chi \\
(P-K) \Phi-\omega \frac{1}{v} \Phi+\left(\sum_{i=1}^{6}\left(\frac{\lambda_{i} \beta_{i}}{\omega+\lambda_{i}} \chi-\beta\right)\right) P \Phi=0
\end{array}\right.
$$

Since $\left(\frac{1}{k_{e f f}} P-K\right) \Phi=0,(P-K) \Phi=\left(1-\frac{1}{k_{\text {eff }}}\right) P \Phi=\rho P \Phi$ the following is obtained: $\rho P \Phi=\left(\omega \frac{1}{v}-\sum_{i=1}^{6}\left(\frac{\lambda_{i} \beta_{i}}{\omega+\lambda_{i}} \chi-\beta_{i}\right) P\right) \Phi$ with the matrix form of the Nordheim equation:

Matrix form of Nordheim equation:

$$
\begin{equation*}
\Phi^{*} \times \rho P \Phi=\Phi^{*} \times\left(\omega \frac{1}{v}-\sum_{i=1}^{6}\left(\frac{\lambda_{i} \beta_{i}}{\omega+\lambda_{i}} \chi-\beta_{i}\right) P\right) \Phi \tag{17.13}
\end{equation*}
$$

In comparison with the point-kinetics model, the $3 D$ effect and the importance are taken into account by weighting with the adjoint flux and integrating over the volumes, which for two energy groups gives:

$$
\bar{\beta}_{i}^{F}=\frac{\beta_{i_{1}}^{F} \int_{\text {volume }} \Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1} d \vec{r}+\beta_{i_{2}}^{F} \int_{\text {volume }} \Phi_{1}^{*} \nu \Sigma_{f_{2}} \Phi_{2} d \vec{r}}{\int_{\text {volume }}\left(\Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f_{2}} \Phi_{2}\right) d \vec{r}}
$$

where $F$ is the index of the fissile system. $\bar{\beta}_{i}$ for the fissile systems composition is obtained by summing over all of these systems:

$$
\bar{\beta}_{i}^{F}=\frac{\sum_{F}\left[\beta_{i_{1}}^{F} \int_{\text {volume }} \Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1} d v+\beta_{i_{2}}^{F} \int_{\text {volume }} \Phi_{1}^{*} \nu \Sigma_{f_{2}} \Phi_{2} d v\right]}{\sum_{F}\left[\int_{\text {volume }}\left(\Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f_{2}} \Phi_{2}\right) d v\right]}
$$

For a core, the integration volume is the core itself, i.e. all the assemblies in it. The total $\bar{\beta}$ is given by $\bar{\beta}=\sum_{i=1}^{6} \bar{\beta}_{i}$. The prompt neutron lifetime is given in (Keepin 1965, p. 165):

$$
\ell=\frac{\int_{\text {volume }} \frac{\Phi_{1}^{*} \Phi_{1}}{v_{1}} d v+\int_{\text {volume }} \frac{\Phi_{2} \Phi_{2}^{*}}{v_{2}} d v}{\int_{\text {volume }}\left(\Phi_{1}^{*} \nu \Sigma_{f_{1}} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f_{2}} \Phi_{2}\right) d v}
$$

The thermal adjoint flux $\Phi_{2}^{*}$ appears in the numerator since:

$$
\ell_{B_{g}}=\frac{\Phi^{*} \times \frac{1}{v} \Phi}{\Phi^{*} \times\left(\Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)\right) \Phi}
$$

from the analogy with $\ell_{B_{g}}=\left[v \Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)\right]^{-1}$, which was shown previously.
$\ell_{0}=\frac{\Phi^{*} \times \frac{1}{v} \Phi}{\Phi^{*} \times \Sigma_{a} \Phi}, \ell=\frac{\ell_{B_{g}}}{k_{e f f}}, k_{e f f}=\frac{\nu \Sigma_{f}}{\Sigma_{a}\left(1+M^{2} B_{g}^{2}\right)}$ where: $\ell_{B_{g}}=\frac{\Phi^{*} \times \frac{1}{v} \Phi}{\Phi^{*} \times \frac{P \Phi}{k_{e f f}}}$
Hence: $\left\{\begin{array}{l}\ell \equiv \frac{\ell_{B_{g}}}{k_{e f f}}=\frac{\Phi^{*} \times \frac{1}{v} \Phi}{\Phi^{*} \times P \Phi} \\ \Phi^{*} \times \frac{1}{v} \Phi=\left[\Phi_{1}^{*}, \Phi_{2}^{*}\right]\left[\begin{array}{l}\frac{1}{v_{1}} \Phi_{1} \\ \frac{1}{v_{2}} \Phi_{2}\end{array}\right]=\Phi_{1}^{*} \frac{1}{v_{1}} \Phi_{1}+\Phi_{2}^{*} \frac{1}{v_{2}} \Phi_{2}\end{array}\right.$

Following the same reasoning, the group-wise $\beta_{\text {eff }}$ for delayed neutrons is given by:
$\bar{\beta}_{i_{e f f}}=\frac{\sum_{F}\left[\beta_{i_{1}}^{F} \int_{\text {volume }} \Phi_{1}^{*}\left(\nu \Sigma_{f_{1}} \Phi_{1}^{\infty}\right) \frac{\Phi_{1}}{\Phi_{1}^{\infty}} \dot{I} d v+\beta_{i_{2}}^{F} \int_{\text {volume }} \Phi_{1}^{*}\left(\nu \Sigma_{f_{2}} \Phi_{2}^{\infty}\right) \frac{\Phi_{2}}{\Phi_{2}^{\infty}} \dot{I} d v\right]}{\sum_{F} \int_{\text {volume }}\left(\Phi_{1}^{*}\left(\nu \Sigma_{f_{1}} \Phi_{1}^{\infty}\right) \frac{\Phi_{1}}{\Phi_{1}^{\infty}}+\Phi_{1}^{*}\left(\nu \Sigma_{f_{2}} \Phi_{2}^{\infty}\right) \frac{\Phi_{2}}{\Phi_{2}^{\infty}}\right) d v}$
where $\dot{I}$ is the importance that includes the delayed neutrons effect (which depend on the fuel type) -of the order of 0.97 for a $P W R . \Phi_{1}^{\infty}, \Phi_{2}^{\infty}$ are the fast and thermal fluxes in an infinite medium, since the real fast and thermal fluxes prevailing in the reactor, $\Phi_{1}, \Phi_{2}$, resulting from a core calculation, are not available in the neutron physics library. $\beta_{\text {eff }}$ is the sum of the group-wise $\beta_{\text {eff }}$ for delayed neutrons:

$$
\bar{\beta}_{e f f}=\sum_{i=1}^{6} \bar{\beta}_{i_{e f f}}
$$

The foregoing shows that the experimental value of $\bar{\beta}_{\text {eff }}$ depends heavily on calculation of the importances and fluxes in an infinite lattice. Recent works ${ }^{14}$ have shown that the $\bar{\beta}_{\text {eff }}$ obtained for $U O X$ and $M O X$ fuel has a $2 \%$ uncertainty within one standard deviation. This is consistent with the criteria required by the Nuclear Energy Agency specialists, who set a 5\% uncertainty level at one standard deviation for industrial reactors.

The Nordheim equation in question is as follows:

$$
\rho=\ell_{B_{g}} \omega+\sum_{i=1}^{6} \frac{\bar{\beta}_{i_{e f f}}}{1+\frac{\bar{\lambda}_{i}}{\omega}}
$$

with:
$\bar{\lambda}_{i}=\frac{\sum_{F}\left[\beta_{i_{1}}^{F} \int_{\text {volume }} \Phi_{1}^{*}\left(\nu \Sigma_{f_{1}} \Phi_{1}^{\infty}\right) \frac{\Phi_{1}}{\Phi_{1}^{\infty}} d v+\beta_{i_{2}}^{F} \int_{\text {volume }} \Phi_{1}^{*}\left(\nu \Sigma_{f_{2}} \Phi_{2}^{\infty}\right) \frac{\Phi_{2}}{\Phi_{2}^{\infty}} d v\right]}{\sum_{F}\left[\frac{\beta_{1}^{F}}{\lambda_{i_{1}}^{F}} \int_{\text {volume }} \Phi_{1}^{*}\left(\nu \Sigma_{f_{1}} \Phi_{1}^{\infty}\right) \frac{\Phi_{1}}{\Phi_{1}^{\infty}} d v+\frac{\beta_{i_{2}}^{F}}{\lambda_{i_{2}}^{F}} \int_{\text {volume }} \Phi_{1}^{*}\left(\nu \Sigma_{f_{2}} \Phi_{2}^{\infty}\right) \frac{\Phi_{2}}{\Phi_{2}^{\infty}} d v\right]}$

[^348]
### 17.11 First-Order Perturbations

A first-order perturbation in a critical reactor causes a change in reactivity of:

$$
d \rho=\frac{\Phi^{*} \times\left(\frac{1}{k_{e f f}} d P-d K\right) \Phi}{\Phi^{*} \times P \Phi}=\frac{\iiint_{\text {Reactor }} \Phi^{*} \times\left(\frac{1}{k_{e f f}} d P-d K\right) \Phi d x d y d z}{\iiint_{\text {Reactor }} \Phi^{*} \times P \Phi d x d y d z}
$$

with $d K \equiv d A-d D \Delta$ since
$K=\left[\begin{array}{cc}\Sigma_{a_{1}}+\Sigma_{r}-D_{1} \Delta & 0 \\ -\Sigma_{r} & \Sigma_{a_{2}}-D_{2} \Delta\end{array}\right]=\left[\begin{array}{cc}\Sigma_{a_{1}}+\Sigma_{r} & 0 \\ -\Sigma_{r} & \Sigma_{a_{2}}\end{array}\right]-\left[\begin{array}{cc}-D_{1} \Delta & 0 \\ & -D_{2} \Delta\end{array}\right]$
If the numerator of the reactivity perturbation is expanded, the following is reached:

$$
\begin{aligned}
\iiint \int_{\text {Reactor }} \Phi^{*} \times\left(\frac{1}{k_{e f f}} d P-d K\right) \Phi d x d y d z= & \iiint_{\text {Reactor }} \Phi^{*} \times\left(\frac{1}{k_{\text {eff }}} d P-d A\right) \Phi d x d y d z \\
& +\iiint_{\text {Reactor }} \Phi^{*} \times d D \Delta \Phi d x d y d z
\end{aligned}
$$

Since: $\operatorname{div}(f \overrightarrow{\operatorname{grad}} \Phi)=f \Delta \Phi+\overrightarrow{\operatorname{grad} f} \times \overrightarrow{\operatorname{grad}} \Phi$ and using the Ostrogradski theorem with the external surface $S$ of the reactor:

$$
\iiint_{\text {Reactor }} \operatorname{div} \vec{k} d x d y d z=\iint_{S} \vec{k} \cdot \vec{n} d S
$$

the following is obtained:

$$
\begin{aligned}
\iiint_{\text {Reactor }} \Phi^{*} \times d D \Delta \Phi d x d y d z= & \iint_{S} \Phi^{*} \times d D \overrightarrow{\operatorname{grad}} \Phi \cdot \vec{n} d S \\
& -\iiint_{\text {Reactor }} \overrightarrow{\operatorname{grad}} \Phi^{*} \times \overrightarrow{\operatorname{grad}} \Phi d D d x d y d z
\end{aligned}
$$

At the external surface of the reactor, the boundary condition linking the diffusion current to the extrapolated length $\lambda$ is used:

$$
\vec{J} \equiv-D \overrightarrow{\operatorname{grad}} \Phi=\frac{\Phi}{3 \lambda} \vec{n}
$$

where:

$$
\iint_{S} \Phi^{*} \times d D \overrightarrow{\operatorname{grad}} \Phi \cdot \vec{n} d S=-\iint_{S} \Phi^{*} \times \frac{d D}{D} \frac{\Phi}{3 \lambda} \cdot \vec{n} d S
$$

Finally:


It should be noted that the surface term is zero in the case of the LefebvreLebigot reflector model used at EDF, which assumes that the diffusion coefficients of the reflector are constant, hence $d D_{\{S\}} \equiv 0$. For two-energy groups, the previous equation is written as:

$$
\begin{array}{r}
\iiint_{\text {Reactor }} \Phi_{1} *\left(\frac{1}{k_{\text {eff }}} \delta \nu \Sigma_{f 1}-\delta \Sigma_{a 1}-\delta \Sigma_{r}\right) \Phi_{1}+\Phi_{1} *\left(\frac{1}{k_{\text {eff }}} \delta \nu \Sigma_{f 2}\right) \Phi_{2} d x d y d z \\
+\iiint_{\text {Reactor }} \Phi_{2}{ }^{*} \delta \Sigma_{r} \Phi_{1} d x d y d z-\iiint_{\text {Refer }} \Phi_{2} \delta \Sigma_{a 2} \Phi_{2} d x d y d z \\
d \rho_{\text {Lefebve-Lebigot }}=\frac{-\iiint_{\text {Reactor }} \delta D_{1} \overrightarrow{g r a d} \Phi_{1} * \overrightarrow{g r a d} \Phi_{1} d x d y d z-\iiint_{\text {Reactor }} \delta D_{2} \overrightarrow{g r a d} \Phi_{2} * \overrightarrow{\operatorname{grad}} \Phi_{2} d x d y d z}{\iiint_{\text {Reactor }}\left(\nu \Sigma_{f 1} \Phi_{1} * \Phi_{1}+\nu \Sigma_{f 2} \Phi_{1}{ }^{*} \Phi_{2}\right) d x d y d z}
\end{array}
$$

In a $2 D$ calculation, the absorption cross sections must be corrected to account for axial leakage. Hence, $\delta \Sigma_{a 1}$ is substituted by $\delta \Sigma_{a 1}+\delta D_{1} B_{1, z}^{2}$ and $\delta \Sigma_{a 2}$ by $\delta \Sigma_{a 2}+\delta D_{2} B_{2, z}^{2}$. As a general rule, the perturbation of cross sections is computed either by the difference between two static calculations with a weakly-perturbed parameter (e.g. temperature, density, boron, xenon, etc.) or by direct derivation (mathematical) if an analytical feedback parameter model is available, as is the case for the Lefebvre-Seban model used at EDF or any interpolation model with known coefficients.

### 17.12 Numerical Reactimeter

The numerical reactimeter (aka reactivity meter) installed in a reactor uses experimental signals which come from the Nuclear Power Chambers (NPC). The latter are inserted in a 0D kinetics model, enabling computation of the doubling time using the following method.

Starting with the two-group kinetics equation (and disregarding up-scattering):

$$
\left\{\begin{array}{l}
\frac{1}{v_{l}} \frac{\partial \Phi_{l}(t)}{\partial t}-D_{l} \Delta \Phi_{l}(t)+\left(\Sigma_{a l}+\Sigma_{l \rightarrow 2}\right) \Phi_{l}(t)=\sum_{F \in\{f i s i l i s\}}\left(1-\beta^{F}\right)\left(\nu \Sigma_{f l}^{F} \Phi_{l}(t)+\nu \Sigma_{f 2}^{F} \Phi_{2}(t)\right)+\sum_{F \in\{f i s i l u s\}} \sum_{g=1}^{G} \lambda_{g}^{F} C_{g}^{F}(t)  \tag{17.14}\\
\frac{1}{v_{2}} \frac{\partial \Phi_{2}(t)}{\partial t}-D_{2} \Delta \Phi_{2}(t)+\Sigma_{a 2} \Phi_{2}(t)=\Sigma_{l \rightarrow 2} \Phi_{l}(t)
\end{array}\right.
$$

The delayed neutron precursors, differentiated for each group $g$ (usually six precursor groups) and for each fissile isotope $i$ (usually a dozen of fissile system), are described by the following equation:

$$
\begin{gather*}
\frac{\partial C_{g}^{F}(t)}{\partial t}=-\lambda_{g}^{F} C_{g}^{F}(t)+\beta_{g}^{F}\left(\nu \Sigma_{f 1}^{F} \Phi_{l}(t)+\nu \Sigma_{f 2}^{F} \Phi_{2}(t)\right)  \tag{17.15}\\
\beta_{g}=\sum_{F \in\{f i s s i l e s\}} \beta_{g}^{F} \quad \beta^{F}=\sum_{g=1}^{G} \beta_{g}^{F} \quad \beta=\sum_{g=1}^{G} \beta_{g}
\end{gather*}
$$

The solutions for the fluxes and concentrations are generally sought in the following form:

$$
\Phi_{1}(t)=\Phi_{1} e^{\omega t}, \Phi_{2}(t)=\Phi_{2} e^{\omega t}, C_{g}^{i}(t)=C_{g}^{i} e^{\omega t}
$$

Equation (17.14) is written as follows using these forms in time:

$$
\left(\omega+\lambda_{g}^{F}\right) C_{g}^{F}=\beta_{g}^{F}\left(\nu \Sigma_{f 1}^{F} \Phi_{1}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)
$$

which, when summed over the groups $g$, leads to:

$$
\sum_{g=1}^{G}\left(\omega+\lambda_{g}^{F}\right) C_{g}^{F}=\sum_{g=1}^{G} \beta_{g}^{F}\left(\nu \Sigma_{f 1}^{F} \Phi_{1}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)=\beta^{F}\left(\nu \Sigma_{f 1}^{F} \Phi_{1}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)
$$

giving:

$$
\begin{aligned}
\sum_{F \in\{\text { fissile }\}} \sum_{g=1}^{G} \lambda_{g}^{F} C_{g}^{F}= & \sum_{F \in\{\text { fissile }\}} \beta^{F}\left(\nu \Sigma_{f 1}^{F} \Phi_{1}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right) \\
& -\omega \sum_{F \in\{\text { fissile }\}} \sum_{g=1}^{G} \frac{\beta_{g}^{F}}{\omega+\lambda_{g}^{F}}\left(\nu \Sigma_{f 1}^{F} \Phi_{1}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)
\end{aligned}
$$

The latter term can be substituted into Eq. (17.14) to give:
$\left\{\begin{array}{l}\frac{1}{v_{l}} \omega \Phi_{l}-D_{1} \Delta \Phi_{l}+\left(\Sigma_{a l}+\Sigma_{l \rightarrow 2}\right) \Phi_{l}=\sum_{F \in\{f \text { sisile }\}}\left(\nu \Sigma_{f 1}^{F} \Phi_{l}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)-\omega \sum_{F \in\{f \text { sisile }\}} \sum_{g=1}^{G} \frac{\beta_{g}^{F}}{\omega+\lambda_{g}^{F}}\left(\nu \Sigma_{f 1}^{F} \Phi_{l}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right) \\ \frac{1}{v_{2}} \omega \Phi_{2}-D_{2} \Delta \Phi_{2}+\Sigma_{a 2} \Phi_{2}=\Sigma_{l \rightarrow 2} \Phi_{l}\end{array}\right.$
This equation can also be expressed as:

$$
\left\{\begin{array}{l}
D_{l} \Delta \Phi_{l}-\left(\Sigma_{a l}+\Sigma_{l \rightarrow 2}\right) \Phi_{l}+\sum_{F \in\{f i s i l l e\}}\left(\nu \Sigma_{f l}^{F} \Phi_{l}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)=\omega\left[\frac{1}{v_{l}} \Phi_{l}+\sum_{F \in\left\{\left\{\text { isisile }^{\prime}\right\}\right.} \sum_{g=1}^{G} \frac{\beta_{g}^{F}}{\omega+\lambda_{g}^{F}}\left(\nu \Sigma_{f l}^{F} \Phi_{l}+\nu \Sigma_{f 2}^{F} \Phi_{2}\right)\right] \\
D_{2} \Delta \Phi_{2}-\Sigma_{a 2} \Phi_{2}+\Sigma_{l \rightarrow 2} \Phi_{l}=\frac{1}{v_{2}} \omega \Phi_{2}
\end{array}\right.
$$

This system of two equations can be written in the form:

$$
(P-K) \Phi=\omega \alpha \Phi
$$

where $P$ and $K$ are the operators defined previously. Using the usual notations, the permanent state is characterized by:

$$
\left(\frac{1}{k_{e f f}} P-K\right) \Phi=0
$$

The scalar product $\Phi^{*} \times$ is applied to these two equations since it contains both the energy aspect (two neutron groups) and the spatial aspect (integration over the volume)

$$
\left\{\begin{array}{l}
\Phi^{*} \times(P-K) \Phi=\Phi^{*} \times \omega \alpha \Phi \\
\Phi^{*} \times\left(\frac{1}{k_{e f f}} P-K\right) \Phi=0
\end{array}\right.
$$

By substitution, the following equation is readily obtained:

$$
\rho \equiv 1-\frac{1}{k_{e f f}}=\omega \frac{\Phi^{*} \times \alpha \Phi}{\Phi^{*} \times P \Phi}
$$

which can be expressed with two energy groups:

$$
\rho=\omega \frac{\iiint_{\text {Reactor }} \frac{\Phi_{1}^{*} \Phi_{1}}{v_{1}}+\frac{\Phi_{2} \Phi_{2}^{*}}{v_{2}} d x d y d z+\iiint_{\text {Reactor }} \sum_{\text {R }\{f \text { fissile }\}} \sum_{g=1}^{G} \frac{\beta_{g}^{F}}{\omega+\lambda_{g}^{F}}\left(\Phi_{1}^{*} \nu \Sigma_{f l}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z}{\iiint_{\text {Reactor }} \sum_{F \in\{f i s s i l e\}}\left(\Phi_{1}^{*} \nu \Sigma_{f 1}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z}
$$

The reactor period is given by $T \equiv \frac{1}{\omega}$ and the doubling time by $T_{d} \equiv \frac{\ln 2}{\omega}$. Using the definitions seen earlier:

$$
\begin{aligned}
\ell & =\frac{\iiint_{\text {Reactor }} \frac{\Phi_{1}^{*} \Phi_{1}}{v_{1}}+\frac{\Phi_{2} \Phi_{2}^{*}}{v_{2}} d x d y d z}{\iiint_{\text {Réactor }} \sum_{F \in\{f \text { fissile }\}}\left(\Phi_{1}^{*} \nu \Sigma_{f 1}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z} \\
\overline{\beta_{g}}= & \frac{\iiint_{\text {Reactor }} \sum_{F \in\{f i s s i l e\}} \beta_{g}^{F}\left(\Phi_{1}^{*} \nu \Sigma_{f 1}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z}{\iiint_{\text {Reactor }} \sum_{F \in\{f i s s i l e\}}\left(\Phi_{1}^{*} \nu \Sigma_{f 1}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z}
\end{aligned}
$$

and:

$$
\overline{\lambda_{g}}=\frac{\iiint_{\text {Reactor }} \sum_{F \in\{f i s s i l e\}} \beta_{g}^{F}\left(\Phi_{1}^{*} \nu \Sigma_{f 1}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z}{\iiint_{\text {Reactor }} \sum_{F \in\{f i s s i l e\}} \frac{\beta_{g}^{F}}{\lambda_{g}^{F}}\left(\Phi_{1}^{*} \nu \Sigma_{f 1}^{F} \Phi_{1}+\Phi_{1}^{*} \nu \Sigma_{f 2}^{F} \Phi_{2}\right) d x d y d z}
$$

Finally, the law linking reactivity and doubling time is obtained:

$$
\rho=\ell \frac{\ln 2}{T_{d}}+\sum_{g} \frac{\overline{\beta_{g}}}{1+\overline{\lambda_{g}} \frac{T_{d}}{\ln 2}}
$$

From this formula, a numerical reactimeter may be defined with coefficients $\ell, \overline{\beta_{g}}, \overline{\lambda_{g}}$ being obtained via 3D core calculation. The doubling time is obtained from measurements registered by power chambers. In France, reactimeters are based on inverse resolution of the point-kinetics equations in which reactivity is given by the solution to the coupled system, with the neutron population, $n(t)$, being taken as the image of the signals measured by the external chambers:

$$
\left\{\begin{array}{l}
\rho(t)=\sum_{g} \overline{\beta_{g}}+\ell \frac{\frac{d n(t)}{d t}-\sum_{g} \overline{\lambda_{g}} C_{g}(t)}{n(t)} \\
\frac{d C_{g}(t)}{d t}=\frac{\overline{\beta_{g}}}{\ell} n(t)-\overline{\lambda_{g}} C_{g}(t)
\end{array}\right.
$$

### 17.13 Practical Evaluation of Prompt Neutron Generation Time

The prompt neutron generation time in a reactor $R$ can be computed in the multigroup formalism ${ }^{15}$ by:

$$
\ell=\frac{\iiint_{R} \sum_{g=1}^{G} \frac{\Phi_{g}^{*} \Phi_{g}}{v_{g}} d V}{\iiint_{R} \sum_{i \in[f i s s i l e s]} \sum_{g=1}^{G} \sum_{h=1}^{G}\left[\left(1-\beta_{i}\right) \chi_{p, g}^{i}+\beta_{i} \chi_{d, g}^{i}\right] \nu_{i} \Sigma_{f}^{i}{ }_{h} \Phi_{g}^{*} \Phi_{h} d V}
$$

where: $G$ is the number of energy groups for the calculation, $\chi_{p, g}^{i}$ is the spectrum of emitted prompt neutrons in group $g$ and by isotope $i, \chi_{d, g}^{i}$ is the spectrum of emitted delayed neutrons in group $g$ and by isotope $i, v_{g}$ is the mean neutron velocity in group $g, \nu_{i} \Sigma_{f h}^{i}$ is the production cross section of isotope $i$ in group $h$, $\Phi_{h}$ is the direct flux in group $h$, and $\Phi_{g}^{*}$ is the adjoint flux (or importance) in group $g$. In a reactor divided into two regions (e.g. with different materials), a summation must be computed over all the regions with different cross sections, fluxes, and neutron velocities. The generation time of prompt neutrons in a reactor may be measured by perturbation (for example, by inserting an absorber at the center of a mock-up reactor). By linearizing the Nordheim equation with respect to the prompt neutron generation time:

$$
\rho=\ell \omega+\sum_{i=1}^{6} \frac{\beta_{i} \omega}{\omega+\lambda_{i}}=\ell \omega(T)+b(T)
$$

The coefficients $\omega(T)$ and $b(T)$ depend on the period of the reactor. Let us assume two states for the reactor, respectively $i$ and $j$ (two peripheral loadings for example). These will be perturbed similarly from a reference state 0 (of measurable period $T_{0}^{i}$ ) to reach a perturbed state $1\left(\right.$ with period $\left.T_{1}^{i}\right)$ :

$$
\Delta \rho_{0 \rightarrow 1}^{i}=\ell\left(\omega_{1}^{i}-\omega_{0}^{i}\right)+\left(b_{1}^{i}-b_{0}^{i}\right)=\Delta \rho_{0 \rightarrow 1}^{j}=\ell\left(\omega_{1}^{j}-\omega_{0}^{j}\right)+\left(b_{1}^{j}-b_{0}^{j}\right)
$$

where: $\ell=\frac{\left(b_{1}^{i}-b_{0}^{i}\right)-\left(b_{1}^{j}-b_{0}^{j}\right)}{\left(\omega_{1}^{j}-\omega_{0}^{j}\right)-\left(\omega_{1}^{i}-\omega_{0}^{i}\right)}$

[^349]In practice, this perturbation is created by inserting a rod with alternating leaded parts, fuel parts enriched at $3.5 \%$ uranium 235 and voided parts in the reactor (of $U N G G$ type with natural uranium). This rod is oscillated up and down as in "oscillation" experiments. The experiment is repeated with $N$ configurations, and the coefficients $\omega(T)$ and $b(T)$ are measured. The values of $\Delta \rho$ are plotted as a function of $\ell$ on the same graph. This leads to a series of plots that cross the abscissa axis at the required $\ell$ being sought, up to the measurement uncertainty. The period of the reactor for a given state is measured by divergence (doubling-time method). For each divergence, several periods are measured, with only the last ones being retained for calibration of the electronic system and for transient problems (Fig. 17.20).


Fig. 17.20 Measurement of generation time of prompt neutrons by perturbation in the Marius pile [From Gérard Gambier: Détermination du temps de vie des neutrons prompts [Determining the life time of prompt neutrons], EDF HF 11/76/73 report (1973)]

The stability of the doubling-time measurement over several periods is an indicator of the reliability of the measured time. The doubling time must be measured to the nearest hundredth of a second for the computation to be sufficiently precise and practically meaningful. A maximum time interval of 0.02 s is therefore allowed between two measurements for a given configuration. In reality, the change in reactivity with the doubling time is not exactly linear, and a slightly longer time interval may be permitted for longer periods (lesser reactivity). If the experiments are carried out at different pressures, corrections to allow for the non-simultaneous effect of pressure on the measurement must be applied in order to bring all the measurements to the same pressure (for small pressure changes, a linear effect of pressure on the doubling time may be assumed). Applied to the Marius reactor with natural uranium fuel, this method resulted in $\ell=0.98 \pm 0.05 \mathrm{~ms}$. The calculation code used at that time predicted $\ell=0.93 \mathrm{~ms}$. This result confirms the 1 ms approximation usually used in $U N G G$ computations.

### 17.14 Main Causes of Reactivity Changes

(Weaver 1968, p. 50)
Below we describe the insertion of reactivity by focusing on the specific physics of water-moderated reactors. In this case, the change in the neutron flux is caused by:

- increased amount of fissile nuclei. This is the case for the loading phase in which assemblies are placed in the core. A mistake during loading can lead to a critical mass of assemblies before loading of the core is complete;
- increased neutron moderation, e.g. by increasing the water density, which enhances neutron thermalization;
- decreased neutron capture in the fuel, e.g. due to a decrease in fuel temperature causing diminished Doppler effect;
- decreased neutron capture in the core by non-fuel materials, e.g. due to ejection of an absorbing rod.


### 17.14.1 Increased Fissile Nuclei

Save for a mistake during the initial reactor design, this situation can occur during loading phases. When the reactor is being loaded, the reactivity is deliberately increased to reach criticality. If an assembly is wrongly positioned, a critical mass can be formed, which is a potential hazard for an "open vessel". For example, and although there were no radiological consequences, an incident of this type occurred during the loading of unit 4 at Dampierre (cycle 18, loading at $2000 \mathrm{MWd} /$ ton owing to an in-cycle shutdown). A mistake during the transfer of an assembly
between the pool in the fuel storage building and the pool in the reactor building led to mispositioning of 114 assemblies (the 25th assembly was not transferred, and its place was occupied by the 26th, and so on until the 139th). In this case, the core remained sub-critical and the reactivity level never exceeded 0.96 . However, had conditions been more unfavorable (BOL core, reduced boron concentration), criticality could have been reached with an open vessel. Since this incident, visual controls have been set up.

### 17.14.2 Increased Neutron Moderation

There may be several reasons for an increase in neutron moderation, either through a decrease in water temperature (increasing the density), an increase in pressure (rise in the number of water molecules in a given volume), or a change in geometry leading to an increase in the local ratio of moderator-to-fuel volumes (assembly flowering, differential temperature dilation, etc.). Of these three reasons, the first is included in the accident studies of uncontrolled power extraction by the secondary loop, which leads to "cold hammering" in the primary loop as in the Steam Line Break. In theory, loss of geometry is controlled by mechanical supports in the assembly (grids, baffle bracers). The risk should thus be negligible for a welldefined core (fast reactors, in which geometry loss leads to high reactivity changes, constitute a separate case, and the solution involves a rigid hexagonal tube binding the assembly and a spacer wire enclosing the fuel pins). The problem of pressure is averted by means of safety valves to ensure a maximum design pressure.

### 17.14.3 Decreased Neutron Capture

There are two types of cause. The first is the negative Doppler effect resulting from uncontrolled cooling of the fuel (triggered by "cold hammering" from a Steam Line Break for example). Causes of the second type are not fuel-related:

- decrease in burnable absorbers like gadolinium,
- decrease in soluble boron concentration (uncontrolled dilution, shown by operational feedback to be far more common in shutdown states than at full power),
- decay in the most absorbing fission product in PWR: xenon-135,
- uncontrolled rod motion (rod ejection, where the effect is more hazardous at zero power due to delayed Doppler feedback).

These causes lead to widely divergent reactivity changes (Table 17.7).

Table 17.7 Main causes of reactivity changes

|  | Speed of reactivity insertion | Magnitude taken in dimensioning studies to account for the phenomenon | Mitigation |
| :---: | :---: | :---: | :---: |
| Dilution of boric acid | $1 \mathrm{pcm} / \mathrm{s}$ | 2000 pcm | - Design of REA and CVCS boration circuits that limit the dilution rate <br> - Protection systems and alarms to inform the operator that action must be taken Remark: The probability of occurrence is much greater during shutdown |
| Extraction of regulating rod banks during normal functioning | $20 \mathrm{pcm} / \mathrm{s}$ | 2000 pcm | - Emergency shutdown with a high power threshold or low DNBR |
| Extraction of regulating rod banks in an abnormal sequence | $100 \mathrm{pcm} / \mathrm{s}$ | 2000 pcm | - Doppler effect is efficient before emergency shutdown |
| Cooling by power extraction via secondary loop (Steam Line Break type) | $100 \mathrm{pcm} / \mathrm{s}$ | 6000 pcm | - Security Injection response <br> - Emergency shutdown with worsening scenario (jammed rod bank) <br> - Operator response required <br> (defective steam generator) |
| Control rod ejection (at zero power, which is the most detrimental since the Doppler Effect is delayed) | $9000 \mathrm{pcm} / \mathrm{s}$ | 900 pcm (worth of the most antireactive rod bank) | - Doppler effect is effective before emergency shutdown |

### 17.15 Reactivity Accident: Insertion of Very High Reactivity Value

Instances of high reactivity insertion are found in accident analysis or "accidentology".

### 17.15.1 Analysis with One Group of Delayed Neutrons

The calculations are simplified by assuming only one group of delayed neutrons. The Nordheim equation is simplified to:
$\rho=\frac{\ell_{B_{g}} \omega}{1+\ell_{B_{g}} \omega}+\frac{1}{1+\ell_{B_{g}} \omega} \frac{\beta \omega}{\omega+\lambda}$ first form of the Nordheim equation
or $\rho=\ell \omega+\frac{\beta_{i} \omega}{\omega+\lambda}$ second form of the Nordheim equation


Fig. 17.21 Nordheim diagram with and without delayed neutrons

In this case, two roots constitute solutions to this equation, but only one of these is positive: $\omega_{0} \gg \omega_{1}$ (and, in the general case, for six delayed neutron groups, $\omega_{0} \gg \omega_{i}$ for i from 1 to 6 ). The stable period of the reactor is given by $T=1 / \omega_{0}$. The flux assumes the following shape $\Phi(r, t)=\Phi_{0}(r) e^{\omega_{0} t}$. If there were no delayed neutrons, the solution to the Nordheim equation would be significantly increased (cf. the dotted line, Fig. 17.21). Since $\omega_{0}>\lambda, \omega_{0}$ can be calculated by simplifying the Nordheim equation:

$$
\rho=\ell \omega_{0}+\frac{\beta_{i} \omega_{0}}{\omega_{0}+\lambda} \approx \ell \omega_{0}+\beta_{i} \text { where: } \omega_{0} \approx \frac{\rho-\beta_{i}}{\ell}=\frac{k_{e f f}(1-\beta)-1}{\ell_{B_{g}}}
$$

In practical cases, $\left|\omega_{1}\right| \ll \frac{1}{\ell_{B_{g}}}$ where: $\rho=\frac{\ell_{B_{g}} \omega}{1+\ell_{B_{g}} \omega}+\frac{1}{1+\ell_{B_{g}} \omega} \frac{\beta \omega}{\omega+\lambda}$
If $\ell_{B_{g}} \omega$ is disregarded with respect to $1, \rho \approx \ell_{B_{g}} \omega+\beta \omega /(\omega+\lambda)$ can be written. The second form of the Nordheim equation is obtained with $\ell_{B_{g}}$ instead of $\ell$. Using the exact second form of the Nordheim equation, the two roots can be computed:

$$
\begin{aligned}
& \ell \omega^{2}+(\ell \lambda+\beta-\rho) \omega-\rho \lambda=0 \quad \Delta=(\ell \lambda+\beta-\rho)^{2}+4 \rho \lambda \ell \\
& \left\{\begin{array}{l}
\omega_{0}=\frac{-(\ell \lambda+\beta-\rho)+\sqrt{(\ell \lambda+\beta-\rho)^{2}+4 \rho \lambda \ell}}{2 \ell} \\
\omega_{1}=\frac{-(\ell \lambda+\beta-\rho)-\sqrt{(\ell \lambda+\beta-\rho)^{2}+4 \rho \lambda \ell}}{2 \ell}<0
\end{array}\right.
\end{aligned}
$$

It should be noted that $\omega_{0}$ may be positive or negative, depending on the sign of $\rho$ (it is in fact of the same sign). If:

$$
\left\{\begin{array}{l}
n(t)=\alpha_{0} e^{\omega_{0} t}+\alpha_{1} e^{\omega_{1} t} \\
C(t)=\gamma_{0} e^{\omega_{0} t}+\gamma_{1} e^{\omega_{1} t}
\end{array} \quad \text { at } \quad t=0:\left\{\begin{array}{l}
n_{0}=\alpha_{0}+\alpha_{1} \\
C_{0}=\gamma_{0}+\gamma_{1}
\end{array}\right.\right.
$$

The concentration of delayed neutrons, initially $C_{0}$, is given by the stationary equation for $t<0$ :

$$
\frac{d C(t)}{d t}=0=\frac{k_{e f f} \beta n_{0}}{\ell_{B_{g}}}-\lambda C_{0}
$$

Thus, the initial concentration: $C_{0}=\frac{k_{e f f} \beta n_{0}}{\ell_{B_{g}} \lambda}=\frac{\beta n_{0}}{\ell \lambda}$. The constant coefficients are coupled by the following conditions:

$$
\left\{\begin{array}{c}
\alpha_{0}+\alpha_{1}=n_{0} \\
\gamma_{0}+\gamma_{1}=\frac{k_{e f f} \beta n_{0}}{\ell_{B_{g}} \lambda}
\end{array}\right.
$$

By inserting $n(t)$ and $C(t)$ in the point-kinetics equations, the coupled differential equation system is obtained:

$$
\begin{gathered}
\left\{\begin{array}{l}
\frac{d n(t)}{d t}=\alpha_{0} \omega_{0} e^{\omega_{0} t}+\alpha_{1} \omega_{1} e^{\omega_{1} t}=\frac{\rho-\beta}{\ell}\left(\alpha_{0} e^{\omega_{0} t}+\alpha_{1} e^{\omega_{1} t}\right)+\lambda\left(\gamma_{0} e^{\omega_{0} t}+\gamma_{1} e^{\omega_{1} t}\right) \\
\frac{d C(t)}{d t}=\gamma_{0} \omega_{0} e^{\omega_{0} t}+\gamma_{1} \omega_{1} e^{\omega_{1} t}=\frac{\beta\left(\alpha_{0} e^{\omega_{0} t}+\alpha_{1} e^{\omega_{1} t}\right)}{\ell}-\lambda\left(\gamma_{0} e^{\omega_{0} t}+\gamma_{1} e^{\omega_{1} t}\right)
\end{array}\right. \\
\left\{\begin{array}{c}
{\left[\alpha_{0} \omega_{0}-\frac{\rho-\beta}{\ell} \alpha_{0}-\lambda \gamma_{0}\right] e^{\omega_{0} t}+\left[\begin{array}{ll}
\left.\alpha_{1} \omega_{1}-\frac{\rho-\beta}{\ell} \alpha_{1}-\lambda \gamma_{1}\right] e^{\omega_{1} t}=0
\end{array}\right.} \\
{\left[\frac{\beta \alpha_{0}}{\ell}-\lambda \gamma_{0}-\gamma_{0} \omega_{0}\right] e^{\omega_{0} t}+\left[\frac{\beta \alpha_{1}}{\ell}-\lambda \gamma_{1}-\gamma_{1} \omega_{1}\right] e^{\omega_{1} t}=0}
\end{array}\right.
\end{gathered}
$$

These two equations are valid for any value of $t$. Thus, the coefficients in front of the exponentials are deduced as being equivalent to zero. The solution of this system of four equations with four unknowns leads to:

$$
\begin{cases}\alpha_{0}=n_{0} \frac{\omega_{1}\left(\lambda+\omega_{0}\right)}{\lambda\left(\omega_{1}-\omega_{0}\right)} & \gamma_{0}=n_{0} \frac{\beta}{\ell \lambda} \frac{\omega_{1}}{\left(\omega_{1}-\omega_{0}\right)}=C_{0} \frac{\omega_{1}}{\omega_{1}-\omega_{0}} \\ \alpha_{1}=-n_{0} \frac{\omega_{0}\left(\lambda+\omega_{1}\right)}{\lambda\left(\omega_{1}-\omega_{0}\right)} & \gamma_{1}=-n_{0} \frac{\beta}{\ell \lambda} \frac{\omega_{0}}{\left(\omega_{1}-\omega_{0}\right)}=-C_{0} \frac{\omega_{0}}{\omega_{1}-\omega_{0}}\end{cases}
$$

Since the product of the roots are given by $\omega_{0} \omega_{1}=-\rho \lambda / \ell$ and their sum worth $\omega_{0}+\omega_{1}=-(\lambda+(\beta-\rho) / \ell)$, the following may be expressed:

$$
\begin{aligned}
& \alpha_{0}=n_{0} \frac{\left(\omega_{1}+\frac{\omega_{0} \omega_{1}}{\lambda}\right)}{\left(\omega_{1}-\omega_{0}\right)}=n_{0} \frac{\left(\omega_{1}-\frac{\rho}{\ell}\right)}{\left(\omega_{1}-\omega_{0}\right)} \text { and } \\
& \alpha_{1}=-n_{0} \frac{\left(\omega_{0}+\frac{\omega_{0} \omega_{1}}{\lambda}\right)}{\left(\omega_{1}-\omega_{0}\right)}=-n_{0} \frac{\left(\omega_{0}-\frac{\rho}{\ell}\right)}{\left(\omega_{1}-\omega_{0}\right)}
\end{aligned}
$$

### 17.15.2 Analysis of the Case of $\rho \gg \beta$ : The Reactivity Accident

Under this hypothesis, the signs of the following coefficients can be predicted as:

$$
\beta+\ell \lambda-\rho<0, \quad \ell \lambda \ll \rho-\beta, 4 \rho \ell \lambda \ll(\beta+\ell \lambda-\rho)^{2}
$$

Using the usual values: the decay constant for a unique group of delayed neutrons is $\lambda \approx 10^{-1} \mathrm{~s}^{-1}$, the prompt neutron lifetime $\ell \approx 2 \times 10^{-5} \mathrm{~s}$, in a PWR. Hence, $\ell \lambda \approx 2 \times 10^{-6}$ or 0.2 pcm . Using a Taylor expansion of the square root: $(1+x)^{1 / 2}=1+x / 2-x^{2} / 8+\ldots$, the roots $\omega_{0}$ and $\omega_{1}$ can be simplified:

$$
\left\{\begin{aligned}
\omega_{0} & \approx \frac{-(\ell \lambda+\beta-\rho)+(\rho-\beta-\overbrace{\ell \lambda}^{\text {negligible }})\left[1+\frac{1}{2} \frac{4 \rho \ell \lambda}{(\rho-\beta-\ell \lambda)^{2}}-\frac{1}{8}\left(\frac{4 \rho \ell \lambda}{(\rho-\beta-\ell \lambda)^{2}}\right)^{2}+\ldots\right]}{2 \ell} \\
& \approx \frac{2(\rho-\beta)+\left[\frac{1}{2} \frac{4 \rho \ell \lambda}{(\rho-\beta)}-\frac{1}{8}\left(\frac{16 \rho^{2} \ell^{2} \lambda^{2}}{(\rho-\beta)^{3}}\right)+\ldots\right]}{2 \ell}=\frac{\rho-\beta}{\ell}+\frac{\rho \lambda}{\rho-\beta}-\frac{\rho^{2} \ell \lambda^{2}}{(\rho-\beta)^{3}}+O\left(\frac{\rho^{3} \ell^{2} \lambda^{3}}{(\rho-\beta)^{5}}\right)
\end{aligned}\right.
$$

where, at the first order: $\quad \omega_{0} \approx \frac{\rho-\beta}{\ell}>0$
Similarly, the second root is given by:
$\omega_{1} \approx \frac{-(\ell \lambda+\beta-\rho)-(\rho-\ell \lambda-\beta)\left[1+\frac{1}{2} \frac{4 \rho \lambda \ell}{(\rho-\beta-\ell \lambda)^{2}}-\frac{1}{8}\left(\frac{4 \rho \ell \lambda}{(\rho-\beta-\ell \lambda)^{2}}\right)^{2}+\ldots\right]}{2 \ell}$
and, finally: $\omega_{1} \approx-\frac{\rho \lambda}{\rho-\beta}+\frac{\rho^{2} \ell \lambda^{2}}{(\rho-\beta)^{3}}-O\left(\frac{\rho^{3} \ell^{2} \lambda^{3}}{(\rho-\beta)^{5}}\right)$
where, at the first order: $\quad \omega_{1} \approx-\frac{\rho \lambda}{\rho-\beta}<0$
To compute the neutron concentration coefficients $\alpha$, the difference between the two roots $\omega_{0}$ and $\omega_{1}$ are determined:

$$
\omega_{1}-\omega_{0} \approx-\frac{\rho \lambda}{\rho-\beta}+\frac{\rho^{2} \ell \lambda^{2}}{(\rho-\beta)^{3}}-\left[\frac{\rho-\beta}{\ell}+\frac{\rho \lambda}{\rho-\beta}-\frac{\rho^{2} \ell \lambda^{2}}{(\rho-\beta)^{3}}\right] \approx-\frac{\rho-\beta}{\ell}-\frac{2 \rho \lambda}{\rho-\beta}
$$

Since $2 \rho \lambda \ell \ll(\rho-\beta)^{2}$, at the first order, the following may be written:

$$
\omega_{1}-\omega_{0} \approx-\omega_{0}=-\frac{\rho-\beta}{\ell}<0
$$

After calculation, this leads to:

$$
\left\{\begin{array}{rl}
\alpha_{0}=n_{0} & \frac{\omega_{1}\left(\lambda+\omega_{0}\right)}{\lambda\left(\omega_{1}-\omega_{0}\right)} \approx n_{0} \frac{\rho}{\rho-\beta}
\end{array}>0\right.
$$

The neutron concentration is given by:
Neutron concentrationduring a reactivity excursion:

$$
\begin{equation*}
n(t)=n_{0}\left(\frac{\rho}{\rho-\beta} e^{\frac{\rho-\beta}{\ell} t}-\frac{\beta}{\rho-\beta} e^{-\frac{\rho \lambda}{\rho-\beta} t}\right) \tag{17.16}
\end{equation*}
$$

It should be noted that for $t=0, n(t=0)=n_{0}$ is obtained despite the simplifications in calculations of roots $\omega_{0}$ and $\omega_{1}$, and of coefficients $\alpha_{0}$ and $\alpha_{1}$, thereby illustrating their valid use. As for the concentration coefficients for the delayed neutrons:

$$
\left\{\begin{aligned}
& \gamma_{0}=C_{0} \frac{\omega_{1}}{\left(\omega_{1}-\omega_{0}\right)} \approx C_{0} \frac{1}{1+\frac{(\rho-\beta)^{2}}{\rho \ell \lambda}}>0 \\
& \gamma_{1}=-C_{0} \frac{\omega_{0}}{\left(\omega_{1}-\omega_{0}\right)} \approx C_{0} \frac{1}{1+\frac{\rho \ell \lambda}{(\rho-\beta)^{2}}}>0
\end{aligned}\right.
$$

The coefficients $\gamma_{0}$ and $\gamma_{1}$ consistently verify that $\gamma_{0}+\gamma_{1}=C_{0}$, despite the simplifications, thus, guaranteeing the initial condition at $t=0$. Therefore, the approximate solutions $n(t)$ and $C(t)$ of the point-kinetics equations are obtained as follows:

High positive reactivity:

$$
\left\{\begin{array}{l}
\Phi(t) \equiv n(t) v=\Phi_{0}\left(\frac{\rho}{\rho-\beta} e^{\frac{\rho-\beta}{\ell} t}-\frac{\beta}{\rho-\beta} e^{-\frac{\rho \lambda}{\rho-\beta} t}\right) \text { with } \Phi_{0} \equiv n_{0} v  \tag{17.17}\\
C(t)=C_{0}\left(\frac{1}{1+\frac{(\rho-\beta)^{2}}{\rho \ell \lambda}} e^{\frac{\rho-\beta}{\ell} t}+\frac{1}{1+\frac{\rho \ell \lambda}{(\rho-\beta)^{2}}} e^{-\frac{\rho \lambda}{\rho-\beta} t}\right)
\end{array}\right.
$$

Assuming that power varies linearly with flux, we have:

$$
P(t)=P_{0}\left(\frac{\rho}{\rho-\beta} e^{\frac{\rho-\beta}{\ell} t}-\frac{\beta}{\rho-\beta} e^{-\frac{\rho \lambda}{\rho-\beta} t}\right)
$$

where $P_{0}$ is the power at the time of injection of reactivity. It will be seen later that this formulation is identical to the case of anti-reactivity insertion (e.g. rod insertion). Following injection of reactivity in the form of a reactivity step, if the neutron concentration is plotted over time, a prompt jump occurs (i.e. a jump caused by the negative term) and decays quickly, thereby reducing the neutron levels from $n_{0}$ to $n_{0} \rho /(\rho-\beta)$. Furthermore, there is no prompt jump for the delayed neutron concentration given that the coefficients of the exponential terms describing $C(t)$ are both positive. At infinity, $n(t)$ and $C(t)$ increase according to the larger (positive) exponential term $e^{\omega_{0} t}$. At $t=0$ :

$$
\frac{d C(t)}{d t}=\gamma_{0} \omega_{0}+\gamma_{1} \omega_{1}=C_{0} \frac{\omega_{1}}{\omega_{1}-\omega_{0}} \omega_{0}-C_{0} \frac{\omega_{0}}{\omega_{1}-\omega_{0}} \omega_{1}=0
$$

The gradient of the delayed neutron concentration is continuous (and zero) at the origin (Fig. 17.22).

### 17.15.3 Insertion of Low Reactivity $0 \leq \rho \ll \beta$

For low reactivity insertion, the following hypotheses are used:

$$
\lambda \ll \frac{1}{\ell}, \quad|\omega| \ll \frac{1}{\ell}, \quad \beta-\rho \approx \beta, \quad \ell \lambda \ll \beta-\rho, \quad \ell \lambda+\beta-\rho>0
$$

Solutions $\omega_{0}$ and $\omega_{1}$ are inverted due to the sign of $\ell \lambda+\beta-\rho$ :


Fig. 17.22 High reactivity step: prompt jump in neutron concentration

$$
\left\{\begin{array}{l}
\omega_{0}=\frac{-(\ell \lambda+\beta-\rho)+\sqrt{(\ell \lambda+\beta-\rho)^{2}-4 \rho \lambda \ell}}{2 \ell} \approx \frac{\rho \lambda}{\beta-\rho}>0 \\
\omega_{1}=\frac{-(\ell \lambda+\beta-\rho)-\sqrt{(\ell \lambda-\beta-\rho)^{2}-4 \rho \lambda \ell}}{2 \ell} \approx-\frac{\beta-\rho}{\ell}<0
\end{array}\right.
$$

The same solutions as for the case of $\rho \gg \beta$ are found, with the indices 0 and 1 inverted.

$$
\omega_{1}-\omega_{0}=\frac{\rho-\beta}{\ell}-\frac{\rho \lambda}{\beta-\rho}=\frac{-(\beta-\rho)^{2}+\rho \lambda \ell}{\ell(\beta-\rho)} \approx-\left(\frac{\beta-\rho}{\ell}\right)
$$

The same applies to the coefficients of the neutron and precursor concentrations:

$$
\left\{\begin{array}{l}
\alpha_{0} \approx n_{0} \frac{\beta}{\beta-\rho} \quad \gamma_{0} \approx C_{0} \frac{1}{1+\frac{\rho \ell \lambda}{(\beta-\rho)^{2}}} \\
\alpha_{1} \approx-n_{0} \frac{\rho}{\beta-\rho} \quad \gamma_{1} \approx C_{0} \frac{1}{1+\frac{(\beta-\rho)^{2}}{\rho \ell \lambda}}
\end{array}\right.
$$

As in the case of the reactivity accident, the same coefficients are obtained, but with the indices 0 and 1 inverted:

Low positive reactivity:

$$
\left\{\begin{align*}
& n(t)=n_{0}\left(\frac{\beta}{\beta-\rho} e^{\frac{\rho \lambda}{\beta-\rho} t}-\frac{\rho}{\beta-\rho} e^{-\frac{\beta-\rho}{\ell} t}\right)  \tag{17.18}\\
& C(t)=C_{0}\left(\frac{1}{1+\frac{\rho \ell \lambda}{(\rho-\beta)^{2}}} e^{\frac{\rho \lambda}{\beta-\rho} t}+\frac{1}{1+\frac{(\rho-\beta)^{2}}{\rho \ell \lambda}} e^{-\frac{\beta-\rho}{\ell} t}\right)
\end{align*}\right.
$$

It should be noted that a prompt jump exists even for a low reactivity insertion.

### 17.16 Anti-reactivity Insertion

In this case, roots $\omega_{0}$ and $\omega_{1}$ are both negative. Usually, $(\ell \lambda+\beta-\rho)^{2} \gg 14 \rho \lambda \ell$, enabling simplification of the roots to:

$$
\left\{\begin{array}{l}
\omega_{0} \approx \frac{-(\ell \lambda+\beta-\rho)+(\ell \lambda+\beta-\rho)\left[1+\frac{4 \rho \lambda \ell}{2(\ell \lambda+\beta-\rho)}\right]}{2 \ell} \approx \frac{\rho \lambda}{\beta-\rho}<0 \\
\omega_{1} \approx \frac{-(\ell \lambda+\beta-\rho)-(\ell \lambda+\beta-\rho)\left[1+\frac{4 \rho \lambda \ell}{2(\ell \lambda+\beta-\rho)}\right]}{2 \ell} \approx \frac{\rho-\beta}{\ell}<0
\end{array}\right.
$$

The root with the most negative value is $\omega_{1}$. The same solutions as for the "low positive reactivity insertion" (previous paragraph) are obtained, and are written using the positive modulus of $\rho$ so as to have positive quantities:

Negative reactivity:

$$
\left\{\begin{align*}
& n(t)=n_{0}\left(\frac{\beta}{\beta+|\rho|} e^{-\frac{|\rho| \lambda}{\beta+|\rho|} t}+\frac{|\rho|}{\beta+|\rho|} e^{-\frac{\beta+|\rho|}{\ell} t}\right)  \tag{17.19}\\
& C(t)=C_{0}\left(\frac{1}{1-\frac{|\rho| \ell \lambda}{(|\rho|+\beta)^{2}}} e^{-\frac{|\rho| \lambda}{\beta+|\rho|} t}+\frac{1}{1-\frac{(|\rho|+\beta)^{2}}{|\rho| \ell \lambda}} e^{-\frac{\beta+|\rho|}{\ell} t}\right)
\end{align*}\right.
$$

A negative prompt jump is seen for the neutron concentration and is even more marked if the inserted reactivity is extremely negative for a negative step. Finally, it


Fig. 17.23 Negative reactivity step: a prompt jump is observed for the neutron concentration, and is more marked as reactivity becomes more negative
should also be noted that the concentration of delayed neutrons cannot decay faster than $\lim _{\rho \rightarrow-\infty} e^{-\frac{|\rho| \lambda}{\beta+|\rho|} t}=e^{-\lambda t}$, which is the radioactive decay for delayed neutron precursors. In other words, while a reactor can be made to diverge as fast as needed by injecting sufficient reactivity, it may be made to converge faster than the natural decay period of the delayed neutron group with the highest decay constant (bromine 87 with a 55.7 s period), and the total fade-out of the fission reaction takes at least 5 min (approximately 10 periods of bromine 87) (Fig. 17.23).

### 17.17 Overview of Cases

We have seen that the solutions of $n(t)$ and $C(t)$ are identical simply with the indices 0 and 1 inverted (assuming that 0 is the index for the positive root). In all three cases (valid for $\rho \gg \beta$ or $\rho \ll \beta$ ), the following can be written:


Fig. 17.24 Nordheim diagram with and without delayed neutrons

Point - kinetics solutions where $\rho$ is not too close to $\beta$ :

$$
\left\{\begin{align*}
& n(t)=n_{0}\left(\frac{\beta}{\beta-\rho} e^{\frac{\rho \lambda}{\beta-\rho} t}-\frac{\rho}{\beta-\rho} e^{-\frac{\beta-\rho}{\ell} t}\right)  \tag{17.20}\\
& C(t)=C_{0}\left(\frac{1}{1+\frac{\rho \ell \lambda}{(\rho-\beta)^{2}}} e^{\frac{\rho \lambda}{\beta-\rho} t}+\frac{1}{1+\frac{(\rho-\beta)^{2}}{\rho \ell \lambda}} e^{-\frac{\beta-\rho}{\ell} t}\right)
\end{align*}\right.
$$

When the inserted reactivity approaches the value of $\beta$, the previous formulae cannot be used (due to the presence of $\rho-\beta$ in the denominator of certain terms). The roots should be expressed without approximation. Graphic analysis of the Nordheim diagram shows that there is no discontinuity at the value of $\omega_{0}$ along the reactivity zone enclosing $\beta$. At most, it increases significantly as $\rho$ approaches $\beta$. In particular, the prompt jump is not related to the fact that $\rho$ is exactly equal to $\beta$ and in reality, it occurs only if $\rho<\beta$ (Fig. 17.24).

### 17.18 Reactivity Step

Let a positive reactivity step be inserted in the core up to a time $T$. Graphical analysis of the previous solutions leads to ( $\rho \ll \beta$ case) (Fig. 17.25):

Suppose that $T$ is much greater than $\ell /(\beta-\rho)$. For $0 \leq t \leq T$, the same results as for a prompt jump are obtained. There is no discontinuity in the gradient of $C(t)$ at the instant when the reactivity changes, which is logical. When criticality is reached


Fig. 17.25 Reactivity step
again $(\rho=0), C(t)$ stabilizes at a new equilibrium state higher than the previous state. The reactivity step is now positive. After $t=T$, the kinetics equations must be solved with $\rho=0$ :

$$
\left\{\begin{array}{l}
\frac{d n(t)}{d t}=-\frac{\beta}{\ell} n(t)+\lambda C(t) \\
\frac{d C(t)}{d t}=\frac{\beta}{\ell} n(t)-\lambda C(t)
\end{array}\right.
$$

The sums of the neutron concentration and of the precursors do not vary with time when reactivity is zero:

$$
\frac{d(n(t)+C(t))}{d t}=0
$$

where: $n(t)+C(t)=C s t=n_{T}+C_{T}$
Finally:

$$
\left\{\begin{array}{c}
n_{T} \approx n_{0} \frac{\beta}{\beta-\rho} e^{\frac{\rho \lambda}{\beta-\rho} T} \\
C_{T} \approx C_{0}\left(\frac{1}{1+\frac{\rho \ell \lambda}{(\rho-\beta)^{2}}} e^{\frac{\rho \lambda}{\beta-\rho} t}+\frac{1}{1+\frac{(\rho-\beta)^{2}}{\rho \ell \lambda}} e^{-\frac{\beta-\rho}{\ell} t}\right) \approx C_{0} e^{\frac{\rho \lambda}{\beta-\rho} T}
\end{array}\right.
$$

The general solution may be found in the form $n(t)=\alpha_{0}+\alpha_{1} e^{\omega(t-T)}$ and $C(t)=\gamma_{0}+\gamma_{1} e^{\omega(t-T)}$. Since $n(t)+C(t)=C s t=n_{T}+C_{T}, \alpha_{1}+\gamma_{1}=0$ :

$$
\begin{gathered}
t=T \quad\left\{\begin{array}{l}
n(t)=n_{T}=\alpha_{0}+\alpha_{1} \\
C(t)=C_{T}=\gamma_{0}+\gamma_{1}
\end{array}\right. \\
\left\{\begin{array}{l}
\frac{d n(t)}{d t}=\alpha_{1} \omega e^{\omega(t-T)}=-\frac{\beta}{\ell}\left(\alpha_{0}+\alpha_{1} e^{\omega(t-T)}\right)+\lambda\left(\gamma_{0}+\gamma_{1} e^{\omega(t-T)}\right) \\
\frac{d C(t)}{d t}=\gamma_{1} \omega e^{\omega(t-T)}=\frac{\beta}{\ell}\left(\alpha_{0}+\alpha_{1} e^{\omega(t-T)}\right)-\lambda\left(\gamma_{0}+\gamma_{1} e^{\omega(t-T)}\right)
\end{array}\right.
\end{gathered}
$$

Which, after calculation, becomes:
Response to a reactivity step:

$$
\left\{\begin{align*}
n(t) & =\frac{\lambda\left(n_{T}+C_{T}\right)}{\lambda+\frac{\beta}{\ell}}+\frac{\frac{\beta}{\ell} n_{T}-\lambda C_{T}}{\lambda+\frac{\beta}{\ell}} e^{-\left(\lambda+\frac{\beta}{\ell}\right)(t-T)}  \tag{17.21}\\
C(t)= & \frac{\beta}{\ell}\left(n_{T}-C_{T}\right) \\
\lambda+\frac{\beta}{\ell} & \frac{\frac{\beta}{\ell}\left(n_{T}-\lambda C_{T}\right)}{\lambda+\frac{\beta}{\ell}} e^{-\left(\lambda+\frac{\beta}{\ell}\right)(t-T)}
\end{align*}\right.
$$

When $t$ tends to infinity, the neutron concentration stabilizes at $\lambda\left(n_{T}+C_{T}\right) /$ $(\lambda+\beta / \ell)$, the precursor concentration stabilizes at $\beta\left(n_{T}+C_{T}\right) / \ell /(\lambda+\beta / \ell)$, and the ratio $C(t) / n(t)$ tends towards $\beta /(\ell \lambda)$. In practice, a reactivity step can simulate the flow of a slug of unborated water (although coarsely if the Doppler effect is disregarded), followed by borated water. Such an incident may occur in the event of problems in the boration circuit (CVCS).

### 17.19 Dropped Control Rod, Insertion of a Large Amount of Anti-reactivity

In the case of an automatic scram or an emergency shutdown of a 900 MWe PWR, dropping of the rod banks $R+G_{1}+G_{2}+N_{1}+N_{2}$ leads to the insertion of antireactivity, depending on the loading pattern at that particular point during the cycle.



Fig. 17.26 Dropping of control rods

This anti-reactivity is estimated at around $\rho=-8000 \mathrm{pcm}$. In this case, with $\beta+\ell \lambda-\rho>0$, which is the same as for the insertion of weak reactivities, but with $\beta-\rho \approx-\rho$, since $|\rho| \gg$, i.e. injection of high reactivity. $4 \rho \lambda \ell \ll(\ell \lambda+\beta-\rho)^{2}$ is still verified (Fig. 17.26):
where: $\omega_{0} \approx \frac{\rho \lambda}{\beta-\rho}<0 \quad \omega_{1} \approx \frac{\rho-\beta}{\ell}<0$
Similarly, the solutions to the point-kinetics model in which $\rho$ is not close to $\beta$, and thus those with insertion of a reactivity step, remain valid. If control rods are dropped, $|\rho|$ is around $5-10 \beta$, therefore, $\omega_{0} \rightarrow-\lambda$. This corresponds to the equations of negative reactivity injection:

$$
\left\{\begin{array}{c}
n(t) \approx n_{0}\left(\frac{\beta}{\beta+|\rho|} e^{-\frac{|\rho| \lambda}{\beta+|\rho|} t}+\frac{|\rho|}{\beta+|\rho|} e^{-\frac{\beta+|\rho|}{\ell} t}\right) \approx n_{0}\left(\frac{\beta}{\beta+|\rho|} e^{-\lambda t}+\frac{|\rho|}{\beta+|\rho|} e^{-\frac{\beta+|\rho|}{\ell} t}\right) \\
C(t) \approx C_{0}\left(\frac{1}{1-\frac{|\rho| \ell \lambda}{(|\rho|+\beta)^{2}}} e^{-\frac{|\rho| \lambda \mid}{\beta+|\rho|} t}+\frac{1}{1-\frac{(|\rho|+\beta)^{2}}{|\rho| \ell \lambda}} e^{-\frac{\beta+|\rho|}{\ell} t}\right) \approx C_{0}\left(\frac{1}{1-\frac{\ell \lambda}{|\rho|}} e^{-\lambda t}+\frac{1}{1-\frac{|\rho|}{\ell \lambda}} e^{-\frac{\beta+|\rho|}{\ell} t}\right)
\end{array}\right.
$$

Core convergence depends on the radioactivity of the delayed neutron group having the longest period, and it cannot be stalled any quicker. A few seconds after the rod drop, the residual power due to the deferred neutrons remains predominant.

### 17.20 Reactivity Ramp

(Hetrick 1993, p. 78; Hummel and Okrent 1970, p. 256; Rozon 1992, p. 174; Stacey 2001, p. 184)

Let us assume that the reactivity takes the form of a ramp function with gradient $\gamma$ after an initial "jump" in amplitude of $\rho_{0}$ (Fig. 17.27):

Fig. 17.27 Reactivity ramp


Starting from the one-group delayed neutron equations:

$$
\left\{\begin{array}{c}
\frac{d n(t)}{d t}=\frac{\rho-\beta}{\ell} n(t)+\lambda C(t) \\
\frac{d C(t)}{d t}=\frac{\beta}{\ell} n(t)-\lambda C(t)
\end{array}\right.
$$

the precursor concentration may be eliminated from these two equations to obtain a second-order equation:

$$
\ell \frac{d^{2} n}{d t^{2}}+\left(\beta-\rho+\lambda \ell \frac{d n}{d t}-\left(\lambda \rho+\frac{d \rho}{d t}\right) n=0\right.
$$

In the case of a ramp, this equation simplifies to:

$$
\frac{d^{2} n}{d t^{2}}+\frac{\left(\beta-\rho_{0}+\lambda \ell-\gamma t\right)}{\ell} \frac{d n}{d t}-\frac{\left(\lambda \rho_{0}+\gamma+\gamma t\right)}{\ell} n=0
$$

which (Hetrick 1993, p. 79) writes out in its canonical form:

$$
\frac{d^{2} n}{d t^{2}}+(A t+B) \frac{d n}{d t}+(C t+D) n=0
$$

Using a mathematical shortcut, this equation may be simplified to a Weber equation. A decomposition, of the form $n(t)=x(t) y(t)$, is written in which $x(t)$ verifies an equation that simplifies the problem. This arbitrary (for the time being) decomposition of $n(t)$ is inserted in the second-order ODE and leads to:

$$
\begin{aligned}
& x \frac{d^{2} y}{d t^{2}}+y \frac{d^{2} x}{d t^{2}}+2 \frac{d x}{d t} \frac{d y}{d t}+(A t+B)\left(x \frac{d y}{d t}+y \frac{d x}{d t}\right)+(C t+D) x y \\
& \quad=x \frac{d^{2} y}{d t^{2}}+y\left[\frac{d^{2} x}{d t^{2}}+(A t+B) \frac{d x}{d t}+(C t+D) x\right]+\frac{d y}{d t}\left[2 \frac{d x}{d t}+(A t+B) x\right]=0
\end{aligned}
$$

Adopting $x(t)$ in particular as the solution of:

$$
2 \frac{d x}{d t}+(A t+B) x=0 \quad \text { i.e. }: x(t) \propto e^{-\frac{(A t+B)^{2}}{4 A}}
$$

allows elimination of the $\frac{d y}{d t}$ term. The $y$ coefficient may then be calculated:

$$
\frac{d^{2} x}{d t^{2}}+(A t+B) \frac{d x}{d t}+(C t+D) x=x\left[-\frac{A^{2}}{4} t^{2}+\left(C-\frac{A B}{2}\right) t+D-\frac{A}{2}-\frac{B^{2}}{4}\right]
$$

allowing the ODE to be simplified to:

$$
\begin{equation*}
\frac{d^{2} y}{d t^{2}}-\left[\frac{A^{2}}{4} t^{2}-\left(C-\frac{A B}{2}\right) t-\left(D-\frac{A}{2}-\frac{B^{2}}{4}\right)\right] y=0 \tag{17.22}
\end{equation*}
$$

The reader will recognize the ODE of the form:

$$
\frac{d^{2} y}{d t^{2}}-\left(a t^{2}+b t+c\right) y=0
$$

the solutions of which are the parabolic cylinder functions deduced from the confluent hypergeometric functions ${ }_{1} F_{1}(a, b, z)$, also known as $M(a, b, z)$ (Abramowitz and Stegun 1972). Using a linear change in variable in time: $t=\alpha \tau+\kappa$, this equation can be written in two different forms ${ }^{16}$ :

$$
\frac{d^{2} y}{d \tau^{2}}-\left(\frac{\tau^{2}}{4}+h\right) y=0 \text { and } \frac{d^{2} y}{d t^{2}}+\left(\frac{\tau^{2}}{4}-h\right) y=0
$$

These equations are called the Weber equations after Heinrich Friedrich Weber (1843-1912). Their solutions are generalized in the form:

$$
\frac{d^{2} D_{n}(x)}{d x^{2}}-\left(\frac{\tau^{2}}{4}-n-\frac{1}{2}\right) D_{n}(x)=0
$$

Further, the parabolic cylinder functions $D_{n}(x)$ are a restriction of the (Edmund T.) Whittaker $W_{k, m}(x)$ functions, and solutions to (Erdélyi 1953, p. 264):

$$
\frac{d^{2} W_{k, m}(x)}{d x^{2}}+\left(-\frac{1}{4}+\frac{k}{x}+\frac{\frac{1}{4}-m^{2}}{x^{2}}\right) W_{k, m}(x)=0
$$

if $D_{n}(x)=\frac{1}{\sqrt{x}} 2^{\frac{n}{2}+\frac{1}{4}} W_{\frac{n}{2}+\frac{1}{4},-\frac{1}{4}}\left(\frac{1}{2} x^{2}\right)$.
Comparing the first form with Eq. (17.20) leads to the following by identification:

[^350]$$
\alpha^{4} a=\alpha^{4} \frac{A^{2}}{4}=\frac{1}{4}
$$

For a positive ramp, $\gamma>0$ and $A>0$, the solution retained is $\alpha^{2} A=-1$ (for a negative gradient, the other solution is kept) such that:

$$
\alpha= \pm \sqrt{-\frac{1}{A}= \pm \sqrt{\frac{\ell}{\gamma}}}
$$

Extending the identification process gives the following:

$$
\left\{\begin{array} { l } 
{ 2 \alpha ^ { 3 } \kappa a + b \alpha ^ { 3 } = 0 } \\
{ \alpha ^ { 2 } b \kappa + c \alpha ^ { 2 } + \alpha ^ { 2 } a \kappa ^ { 2 } = h }
\end{array} \text { hence: } \left\{\begin{array}{l}
\kappa=\frac{2 C-A B}{A^{2}}=\frac{\ell}{\gamma}\left(\frac{\beta-\rho}{\ell}-\lambda\right) \\
h=-\frac{1}{2}+\frac{D}{A}-\frac{C B}{A^{2}}+\frac{C^{2}}{A^{3}}=\frac{1}{2}+\frac{\lambda \beta}{\gamma}
\end{array}\right.\right.
$$

where:

$$
\frac{d^{2} y}{d \tau^{2}}-\left(\frac{\tau^{2}}{4}+\frac{1}{2}+\frac{\lambda \beta}{\gamma}\right) y=0 \quad \text { with: } t= \pm \sqrt{\frac{\ell}{\gamma} \tau}+\frac{\ell}{\gamma}\left(\frac{\beta-\rho}{\ell}-\lambda\right)
$$

the solution of which is the parabolic cylinder function $D_{-1-\lambda \beta / \gamma}(\tau)$ of order $\nu=-1-\lambda \beta / \gamma$-it is tabulated or expanded in Taylor series in some mathematical references ((Abramowitz and Stegun 1972) or as a function of Mathematica). Hetrick (1993, p. 81) points out that where $\nu$ is an integer (negative), $D_{n}(x)$ reduces to a Hermite function, i.e. $\varphi_{n}(x)=H_{n}(x) e^{-x^{2} / 2}$ where $H_{n}(x)$ are the Hermite polynomials ${ }^{17}$ of degree $n$. The response of $n(t)$ to a ramp function can be computed using simpler functions (e.g. error function, exponential function, etc.). For example, (Hetrick 1993) gives the following analytical results:

$$
\left\{\begin{array}{c}
\frac{n(t)}{n_{0}}=e^{\frac{\gamma}{2 t^{2}}-\frac{\beta_{\ell}}{\ell^{t}}\left(1+\beta \sqrt{\frac{\pi}{2 \gamma \ell}} e^{\frac{\beta^{2}}{2 \lambda}}\left(e r f\left(\frac{\beta}{\sqrt{2 \gamma \ell}}\right)-e r f\left(\frac{\beta-\gamma t}{\sqrt{2 \gamma \ell}}\right)\right)\right) \quad \frac{\lambda \beta}{\gamma}=0, \rho_{0}=0} \\
\frac{n(t)}{n_{0}}=\frac{\beta^{2}}{\gamma \ell}\left[e^{-\lambda t}-\frac{\beta-\lambda \ell-\gamma t}{\beta} e^{\frac{\gamma}{2 \ell} t^{2}-\frac{\beta}{\ell} t}\left(1+\beta \sqrt{\left.\left.\frac{\pi}{2 \gamma \ell} e^{\frac{(\beta-\lambda)^{2}}{2 \gamma \ell}}\left(\operatorname{erf}\left(\frac{\beta-\lambda \ell}{\sqrt{2 \gamma \ell}}\right)-e r f\left(\frac{\beta-\lambda \ell-\gamma t}{2 \gamma \ell}\right)\right)\right)\right]}\right.\right. \\
\frac{\lambda \beta}{\gamma}=1, \rho_{0}=0
\end{array}\right.
$$

The first formula is used in cases of high ramps with $\lambda \beta / \gamma \ll 1$ (reactivity accident).

[^351]
### 17.21 Reactivity Transient

For illustration purposes, a reactivity transient at low power (of the order of a mW ) is shown. This negligible power level ensures that there will be no temperature effect on the core behavior (the Doppler effect, which decreases reactivity when power increases thereby heating the fuel). In addition, this also allows observation of the core behavior as pure exponential functions following the prompt jumps, which appear with each increase or decrease in reactivity (Fig. 17.28).

In the particular case of a decrease in reactivity from +100 pcm to +50 pcm , it may be seen that even if the reactivity remains positive, the power decreases during the prompt jump to follow an exponential that grows more slowly than in the case of +100 pcm . This effect is contrary to the widespread idea: "power increases when reactivity is positive". It also depends on the prompt and on delayed neutron concentrations, and on any changes therein before the reactivity jump. Soon after the reactivity transient, this maxim is verified.

### 17.22 Power Excursion

When a large amount of reactivity is inserted accidentally, initially, the power behaves exponentially provided that the core does not heat up, and the Doppler effect begins, halting the power excursion. In the 1940s, relatively simple models were set up to determine the energy released during a power pulse.

Fig. 17.28 Core behavior at low power due to changes in reactivity


Photo 17.3 (a) Lothar Nordheim (left) et (b) Klaus Fuchs (right) (Public domain)
a

b


### 17.22.1 The Nordheim-Fuchs Model

The model developed by Lothar Nordheim and Klaus Fuchs (1911-1988) ${ }^{18}$ in 1946 assumes that the neutron population varies exponentially and disregards the effect due to delayed neutrons (Hetrick 1993, p. 164; Lewins 1978, p. 201; Hummel and Okrent 1970, p. 258; Rozon 1992, p. 296), R. Scalettar in (Weaver 1964, p. 254; Weisman 1977, p. 411) (Photo 17.3):

$$
\frac{d n}{d t} \approx \frac{\rho-\beta}{\ell} n(t)
$$

The difference $\rho-\beta$ is sometimes referred to as prompt reactivity [ $\rho_{p}$ in Rozon (1992)]. The contribution of delayed neutrons is disregarded. The cause of the accident is considered to be a reactivity step, $\rho_{0}$, that is counterbalanced by Doppler feedback, modeled by $-\alpha_{D}\left(T-T_{r e f}\right)$, where $\alpha_{D}$ is the Doppler coefficient in $p c m / K$ and $T-T_{r e f}$ the difference in temperature with respect to the reference temperature at the beginning of the accident. Reactivity obeys a law of the form:

$$
\begin{equation*}
\text { Doppler feedback: } \rho(t)=\rho_{0}-\alpha_{D}\left(T-T_{r e f}\right) \tag{17.23}
\end{equation*}
$$

This type of behavior is suitable for modeling control rod ejection, where the reactivity is injected almost instantaneously (the rod is removed from its position by a sudden fall in pressure caused by disruption of the control casing, which leads to a pressure difference of approximately 150 bars between the top and the bottom of the core in a $P W R$ ). The force and speed of the event is such that power cannot be easily transferred to the moderator for cooling, particularly since the heat flux far

[^352]exceeds the critical flux, and a steam film isolates the fuel. The accident is assumed to be quasi-adiabatic, hence leading (Hetrick 1993, p. 161) to write:
$$
\rho_{U O_{2}} C_{p}^{U O_{2}} \frac{d T}{d t} \approx q_{\left[W / m^{3}\right]}=\kappa \Sigma_{f} \Phi \equiv \kappa \Sigma_{f} n(t) v
$$
which may be expressed more concisely as: $\frac{d T}{d t}=K n(t)$
If the accident cannot be considered adiabatic, the temperature at a given point in the reactor will depend on the temperatures in the other zones, and hence, on neutron density. This model is no longer applicable. The change in reactivity over time can be calculated by setting:
$$
\frac{d \rho}{d t}=\frac{d \rho}{d T} \frac{d T}{d t}=-\alpha K n(t)
$$

Suppose that $\frac{d n}{d \rho} \approx \frac{d n}{\frac{d t}{d \rho}}, \frac{d n}{d \rho}=-\frac{\rho-\beta}{\alpha K \ell}$ is obtained and can be easily integrated as:

$$
n(\rho)=C s t-\frac{(\rho-\beta)^{2}}{2 \alpha K \ell}
$$

If the initial value is such that the amount of neutrons is small, i.e. $n\left(\rho_{0}\right) \approx 0$, the constant term is approximately:

$$
n(\rho) \approx \frac{\left(\rho_{0}-\beta\right)^{2}}{2 \alpha K \ell}-\frac{(\rho-\beta)^{2}}{2 \alpha K \ell}
$$

The maximum of $n(t)$ is reached when its time derivative, $d n / d t$, is zero, which is when $\rho=\beta$, in other words when the reactor is prompt critical. At this point, the Doppler and thermal-hydraulic feedbacks will stop the accident. The maximum neutron concentration, and thus power, is worth the following with a first-order approximation:

$$
n_{\max (\rho=\beta)}=\frac{\left(\rho_{0}-\beta\right)^{2}}{2 \alpha K \ell}
$$

It should be noted that the plot of $n(\rho)$ is parabolic and symmetrical with respect to the maximum point. The frequency $\omega_{0}=\left(\rho_{0}-\beta\right) / \ell$ of the prompt jump owing to a reactivity step of $\rho_{0}$ can be written in the formula. This reactivity step drives the power excursion in time at the beginning of the accident. The accident ends when the neutron population becomes negligible, which is when $\rho\left(t_{\text {fin }}\right)-\beta=-\left(\rho_{0}-\beta\right)$. This is the point at which the parabola is once again worth zero. The increase in fuel temperature is:

$$
T_{\text {fin }}-T_{\text {ref }}=\frac{\rho_{0}-\rho\left(t_{\text {fin }}\right)}{\alpha_{D}}=\frac{2\left(\rho_{0}-\beta\right)}{\alpha_{D}}
$$

In adiabatic cases, the energy released by the power excursion is computed as:
Nordheim - Fuchs model: $\Delta E=\frac{T_{\text {fin }}-T_{r e f}}{K}=\frac{2\left(\rho_{0}-\beta\right)}{\alpha_{D} K}$
This very simple model gives a quick estimate of the power peak and the total energy released. The latter is proportional to the difference between the initial reactivity and the delayed neutron fraction, and is inversely proportional to the Doppler coefficient. This explains the importance of these two parameters. Further, reactivity can be integrated with respect to time since:

$$
\frac{d \rho}{d t}=-\alpha K n(\rho)=-\frac{\left(\rho_{0}-\beta\right)^{2}}{2 \ell}+\frac{(\rho-\beta)^{2}}{2 \ell}
$$

the integration of which is simplified by assuming that the time basis starts at the moment of the power peak, i.e.:

$$
\rho(t)=\beta-\left(\rho_{0}-\beta\right) \operatorname{th}\left(\frac{\left(\rho_{0}-\beta\right) t}{2 \ell}\right)
$$

$1 / \omega_{0}=\ell /\left(\rho_{0}-\beta\right)$ is sometimes called the asymptotic relaxation of the reactor (Weaver 1964, p. 254). The neutron concentration is obtained by:

$$
n(t)=-\frac{1}{\alpha K} \frac{d \rho}{d t}=\frac{1}{\alpha K}\left[\frac{\left(\rho_{0}-\beta\right)^{2}}{2 \ell}+\frac{(\rho-\beta)^{2}}{2 \ell}\right]=n_{\max (\rho=\beta)} \sec \mathrm{h}^{2}\left(\frac{\left(\rho_{0}-\beta\right) t}{2 \ell}\right)
$$

This proves that the power of the reactor can be written in the form of:

$$
P(t)=P_{\max \left(\rho=\beta, t=t_{\max }\right)} \sec h^{2}\left(\frac{\left(\rho_{0}-\beta\right)\left(t-t_{\max }\right)}{2 \ell}\right)
$$

Finally, the energy released, $E(t)=\int_{t_{0}}^{t} P\left(t^{\prime}\right) d t^{\prime}$, which is the integral of the power, is written as (Fig. 17.29):

$$
E(t)=\frac{\left(\rho_{0}-\beta\right)}{\alpha_{D} K}\left[1+\operatorname{th}\left(\frac{\left(\rho_{0}-\beta\right) t}{2 \ell}\right)\right]
$$

The practical width of the pulse at mid-height is $3.52 / \omega_{0}$ and the position of the power peak is given by:

Fig. 17.29 Symmetrical pulse in Nordheim-Fuchs theory


$$
t_{\max }-t_{0}=\frac{1}{\omega_{0}} \ln \left(\frac{4 P_{\max }}{P_{0}}\right)
$$

In this approach, no properties pertaining to delayed neutrons are used (since they are disregarded) other than the fraction $\beta$. This reasoning is valid only for a characteristic period of the accident worth $\Delta E / n_{\max (\rho=\beta)}=4 / \omega_{0}$, which is fairly small compared to the shortest period for a delayed neutron group, itself worth 0.2 s. Beyond this period, the delayed neutrons must be taken into account and the adiabatic hypothesis revised. Further, for an actual reactor, very large reactivity can excite the higher fundamental modes. In (Weaver 1964), Scaletar developed a flux expansion on the eigenmodes, which corrects the Nordheim-Fuchs model by integrating space effects. If assuming that a reactivity step of taken reactivity $\rho_{0}$ to make the reactor prompt critical is too coarse, a reactivity ramp may be used such that:

$$
\rho-\beta=\gamma\left(t-t_{p c}\right)
$$

$t_{p c}$ is the time when the reactor becomes prompt critical (Rozon 1992, p. 187). This makes the shift in the time basis very simple: $\tau \equiv t-t_{p c}$ to solve the prompt-critical equation:
$\frac{d n(\tau)}{d \tau}=\frac{\rho(\tau)-\beta}{\ell} n(\tau)$ with the following initial value: $\rho(\tau=0)=\beta$
Assuming a reactivity ramp, integration of this equation leads to:

$$
n(t)=n\left(t_{p c}\right) e^{\frac{\gamma}{2 t}\left(t-t_{p c}\right)^{2}} \text { with } t_{p c} \approx \frac{\beta}{\gamma}
$$

The previous exact calculations for the ramp suggest that $n\left(t_{p c}\right) \approx 2 n_{0} \sqrt{\frac{\pi}{2 \gamma \ell}}$.
The Nordheim-Fuchs model is useful on account of its technical simplicity. Improvements were proposed in the 1950s such as taking into account the linear dependence of the heat capacity and the differential Doppler coefficient varying with temperature, and in particular, delayed neutrons for slower accidents, by calculating the following perturbation:
with:

$$
\begin{gathered}
\delta n=\frac{1}{\ell} \int \sum \lambda_{i} C_{i} \\
C_{i}(t)=C_{i}(0) e^{-\lambda_{i} t}+\beta_{u} e^{-\lambda_{i} t} \int_{0}^{t} n(\tau) e^{+\lambda_{i} \tau} d \tau
\end{gathered}
$$

$$
\approx C_{i}(0) e^{-\lambda_{i} t}+\beta_{u} e^{-\lambda_{i} t} \int_{0}^{t} n_{\max \left(\rho=\beta, t=t_{\max }\right)} \operatorname{sech}^{2}\left(\frac{\left(\rho_{0}-\beta\right)\left(\tau-t_{\max }\right)}{2 \ell}\right) e^{+\lambda_{i} \tau} d \tau
$$

In this approach, ${ }^{19}$ the precursor concentration is computed using the solution to the Nordheim-Fuchs model without the delayed neutrons to compute the first-order perturbation $\delta n$ (Fig. 17.30).

### 17.22.2 The Chernick Model

J. Chernick, from Brookhaven National Laboratory, models ${ }^{20}$ the effect of the core temperature on neutron kinetics end of 1951. Equations are written as follow:

[^353]

Fig. 17.30 High power excursion in a fast-neutron reactor under the influence of a reactivity ramp of $d k_{\text {eff }} / d t=6.4 \mathrm{~s}^{-1}$ [adapted from (Hummel and Okrent 1970, p. 278)]

$$
\frac{d n(t)}{d t}=\frac{\left(k_{e f f}-1\right) n(t)}{\ell}
$$

Parameter $\ell$ is the mean generation time taking into account the delayed neutrons. The dependence of reactivity versus temperature is modelled through a linear law, wich origin is the ambiant temperature $\left(20^{\circ} \mathrm{C}\right)$. It should be noted that the model uses a so-called "core temperature", without discriminazing between fuel and water moderator:

$$
k_{e f f}\left(T_{[K]}\right)=k_{e f f}\left(T=293_{[K]}\right)-\alpha_{T}\left(T_{[K]}-293 K\right)
$$

Therefore of course:
Core temperature feedback:

$$
\begin{equation*}
k_{\text {eff }}\left(T_{[K]}\right)-1=\underbrace{k_{\text {eff }}\left(T=293_{[K]}\right)-1}_{k_{\text {exc }}}-\alpha_{T}\left(T_{[K]}-293 K\right) \tag{17.25}
\end{equation*}
$$

A distinction between water and fuel would lead to a same distinction between differential coefficients $\alpha_{\text {mod }}$ and $\alpha_{f u e l}$. New parameter $k_{\text {exc }}$ is an image of the reactivity of the cold state of the reactor. The variation of the core temperature is govern by a differential equation taking into account the power released, allegedly supposed linear to the number of neutrons, and a "relaxation" constant $\lambda$ due to the cooling of the fuel by water:

Thermal behaviour of the reactor: $\frac{d T(t)}{d t}=\gamma n(t)-\lambda(T(t)-293 K)$
Two steady solutions are possible $\left(\alpha_{T}>0, \lambda>0\right)$ :

$$
n(t=+\infty)=0, \quad T(t=+\infty)=293 K, \quad k_{e f f}(t=+\infty)=k_{e f f}\left(T=293_{[K]}\right)
$$

which is a perfect cooling down to ambiance, and the asymptotic solution:

$$
n(t=+\infty)=\frac{\lambda k_{e x c}}{\alpha_{T} \gamma}, \quad T(t=+\infty)-293 K=\frac{k_{e x c}}{\alpha_{T}}
$$

Deriving the temperature differential equation with respect to time and by eliminating the neutron concentration in the resulting second order equation, leads to:

$$
\frac{d^{2} T(t)}{d t^{2}}+\left(\lambda-\frac{k_{e x c}}{\ell}\right) \frac{d T(t)}{d t}-\lambda \frac{k_{e x c}}{\ell} T(t)=-\frac{\alpha_{T}(T(t)-293 K)}{\ell}\left(\frac{d T(t)}{d t}+\lambda(T(t)-293 K)\right)
$$

Non-linear terms were left on the right-side member of the equation, wich can be further simplified using:

$$
\varpi_{0} \equiv \frac{k_{e x c}}{\ell}
$$

Therefore:

$$
\frac{d^{2} T(t)}{d t^{2}}+\left(\lambda-\varpi_{0}\right) \frac{d T(t)}{d t}-\lambda \varpi_{0} T(t)=-\frac{\alpha_{T}(T(t)-293 K)}{\ell}\left(\frac{d T(t)}{d t}+\lambda T(t)\right)
$$

A close mathematical analysis of this equation shows that, with a positive temperature coefficient ( $\alpha_{T}<0$ ), divergent temperature solutions occurs, with only stable solutions when $\varpi_{0}<0$ (very low initial $k_{\text {eff }}$, whereas a negative temperature coefficient ( $\alpha_{T}>0$ ) produces convergent solutions, sometimes oscillating around the asymptot $T_{\infty}$ (depending on the value of $\varpi_{0}$ ). Chernick writes the equation under adimensional form and analyses the stability with the help of a phase diagram (adimensional temperature versus adimensional derivate of the temperature). Singular and saddle points occur, depending on the value of the different physical parameters.

### 17.22.3 The Bethe-Tait Model

(Hetrick 1993, p. 223; Hummel and Okrent 1970, p. 263)
In 1956, Hans Bethe (1906-2005) and J. H. Tait proposed a model for the energy released in fast reactors based on a first-order perturbation approach for the diffusion equation with one energy group (Weisman 1977, p. 417) (Photo 17.4).

The fast reactors have short generation times and may undergo mechanical core compaction under accidental conditions. The very fast power excursion can lead to fusion of the core, or even vaporization of the fuel. Fusion of the fuel leads to compaction of the core in the lower parts of the vessel by gravitational pull. This may cause an increase in reactivity of up to 50 Dollars per second! Above a given threshold, the pressure generated by the accident and the energy released are considered to be linked by a linear formula. The temperature effects are due only to pressure gradients. If an ideal reactivity excursion with a $\rho=\beta+\gamma t$ ramp function and without feedback effects is considered such that the reactor is prompt critical at $t=0$, the neutron population obeys the following growth law (Hetrick 1993, p. 223):

Photo 17.4 The renowned 1956 Risley RHM(56)113 report (declassified) by H. Bethe and J. H. Tait: "An estimate of the order of magnitude of vigorous interaction expected should the core of a fast reactor collapse" (Public domain)


$$
\frac{d n}{d t}=\frac{\gamma t}{\ell} n \text { thus, } n(t)=n\left(t_{p c}\right) e^{\frac{\gamma t^{2}}{2 \ell}}
$$

The energy released is proportional to the integral of the power $P(t)$, which is directly proportional to this neutron population:

$$
E(t)=\int_{0}^{t} P(\tau) d \tau=P\left(t_{p c}\right) \int_{0}^{t} e^{\frac{\gamma t^{2}}{2 \ell}} d \tau
$$

It may be seen that this expression contains the error function. For $\gamma t^{2} /(2 \ell) \gg 1$, the following may be written:

$$
E(t) \propto n\left(t_{p c}\right) \frac{\ell}{\gamma t} e^{\frac{\gamma t^{2}}{2 \ell}}
$$

If a threshold of released energy is fixed at $E_{\text {threshold }}$, the time taken to reach this value is given by the transcendental equation:

$$
\frac{\gamma t_{\text {threshold }}^{2}}{\ell}=\ln \left(\frac{\gamma t_{\text {threshold }} E_{\text {threshold }}}{\ln \left(t_{p c}\right)}\right)^{2}
$$

At this threshold energy, the excess pressure leads to a loss in geometry which returns the reactivity to $\beta$. This threshold was calculated by Bethe-Tait as being worth $10^{5} \mathrm{~J} / \mathrm{kg}$. Numerically, it may be seen that the excursion is more severe if the accident starts at low power, since reactivity will have more time to increase before reaching the threshold. Another explanation, not apparent in this model, is that the Doppler effect will be delayed due to the thermal inertia of the fuel if the accident occurs at low power, when the fuel is "cold". The excess energy $E(t)-E_{\text {threshold }}$ generates pressure that induces mechanical stress such that the fuel moves towards the over-critical zone to decrease the reactivity.

Assuming that the flux obeys a one-energy group diffusion equation:

$$
-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi)+\Sigma_{a} \Phi=\nu \Sigma_{f} \Phi
$$

Since $\Sigma_{a}=\Sigma_{c}+\Sigma_{f}$, the first-order perturbation owing to the change in the diffusion coefficient is written as:

$$
\delta k_{e f f}=k_{e f f}-k_{e f f}^{0}=\frac{\int_{\text {Reactor }}\left[-\delta D(\overrightarrow{\operatorname{grad} \Phi} \Phi)^{2}+\left((\nu-1) \delta \Sigma_{f}-\delta \Sigma_{c}\right) \Phi^{2}\right] d r^{3}}{\int_{\text {Reactor }} \nu \Sigma_{f} \Phi^{2} d r^{3}}
$$

In this formula, $k_{\text {eff }}^{0}$ represents the reactivity immediately after the reactivity injection that caused the accident. The adjoint flux is usually included in the perturbation formula but, for a fast reactor, the fast direct flux provides a good estimate of the adjoint flux. In a one-energy group calculation, the appropriatelynormalized adjoint flux is exactly equal to the direct flux. Nonetheless, the weighting of the diffusion coefficient by the square of the flux gradient is not a formal justification (Hetrick 1993, p. 225). The increase in reactivity due to core compaction, equivalent to an increase in material densities, $\rho_{c}$, is described by the differential efficiency of compaction of the core materials, $W_{c}(r)$. The global effect is obtained by summing over the reactor volume:

Compaction effect: $k_{\text {eff }}-k_{\text {eff }}^{0}=\int_{\text {Reactor }} \delta \rho_{c} W_{c}(r) d r^{3}$
The change in density is caused by the shift in fuel position, i.e.:

$$
\delta \rho_{c}=-\operatorname{div}\left(\rho_{c} \vec{u}\right)
$$

where $\vec{u}$ is the shift that is not uniform in all directions. This expression is substituted in Eq. (17.23) and the result integrated by parts:

$$
k_{e f f}-k_{e f f}^{0}=\int_{\text {Reactor }} \rho_{c} \vec{u} \vec{W}_{c}(r) d r^{3}
$$

The effects of this shift on the physical properties of the fuel are given by:

$$
\left\{\begin{array}{l}
\delta \Sigma_{f}=-\operatorname{div}\left(\Sigma_{f} \vec{u}\right) \\
\delta \Sigma_{c}=-\operatorname{div}\left(\Sigma_{c} \vec{u}\right) \\
\delta D=\operatorname{div}(D \vec{u})-2 \vec{u} \cdot \overrightarrow{g r a d} D
\end{array}\right.
$$

These are substituted in the perturbed equation and the divergence terms are integrated by parts to eliminate $\vec{u}$, giving:

$$
\begin{aligned}
\delta k_{\text {eff }} & =k_{\text {eff }}-k_{\text {eff }}^{0} \\
& =\frac{\int_{\text {Reactor }} \vec{u} \cdot\left[2 \overrightarrow{\operatorname{grad}}\left(D(\overrightarrow{\operatorname{grad} \Phi} \Phi)^{2}\right)+D \overrightarrow{\operatorname{grad}}\left((\overrightarrow{\operatorname{grad} \Phi})^{2}\right)-2 \overrightarrow{\operatorname{grad} \Phi \operatorname{divD} \overrightarrow{\operatorname{grad} \Phi}] d^{3} r}\right.}{\int_{\text {Reactor }} \nu \Sigma_{f} \Phi^{2} d^{3} r}
\end{aligned}
$$

which may be simplified to:

$$
\begin{aligned}
\delta k_{\text {eff }} & =k_{\text {eff }}-k_{\text {eff }}^{0} \\
& =\frac{\int_{\text {Reactor }} \vec{u} \cdot\left[\frac{1}{D} \overrightarrow{\operatorname{grad}}\left((D \overrightarrow{\operatorname{grad}} \Phi)^{2}\right)-2 \overrightarrow{\operatorname{grad}} \Phi \operatorname{div}(D \overrightarrow{\operatorname{grad} \Phi})\right] d^{3} r}{\int_{\text {Reactor }} \nu \Sigma_{f} \Phi^{2} d^{3} r}
\end{aligned}
$$

This formula can be compared to Eq. (17.23) using the differential efficiency $W$ such that:

$$
k_{e f f}-k_{e f f}^{0}=\int_{\text {Reactor }} \rho_{c} \vec{u} \vec{W}(r) d^{3} r
$$

with
First-order perturbationof neutron properties:

$$
\begin{equation*}
\vec{W}=\frac{\overrightarrow{\operatorname{grad}}\left((D \overrightarrow{\operatorname{grad}} \Phi)^{2}\right)-2 \overrightarrow{\operatorname{grad}} \Phi \operatorname{div}(\mathrm{D} \overrightarrow{\operatorname{grad}} \Phi)}{\rho_{c} D \int_{\text {Reactor }} \nu \Sigma_{f} \Phi^{2} d^{3} r} \tag{17.28}
\end{equation*}
$$

which may be determined for simple types of geometries of the following form (see Table 17.8):

$$
W=-\frac{\alpha}{r D \rho_{c}} \frac{\left(D \frac{d \Phi}{d r}\right)^{2}}{\int_{\text {Reactor }} \nu \Sigma_{f} \Phi^{2} d^{3} r}
$$

The kinetics equation linking displacement and pressure is given by:

$$
\rho_{c} \frac{d^{2} \vec{u}}{d t^{2}}=-\overrightarrow{\operatorname{grad}} p
$$

Deriving Eq. (17.24) twice with respect to time gives the following:

$$
\frac{d^{2} k_{e f f}}{d t^{2}}=\int_{\text {Reactor }} p d i v \vec{W} d^{3} r
$$

Table 17.8 Form parameter of differential efficiency

|  | Slab reactor | Infinite cylindrical reactor | Spherical reactor |
| :--- | :--- | :--- | :--- |
| $\alpha$ | 0 | 2 | 4 |

Bethe and Tait considered that the spatial shape of the flux and power obeyed a parabolic law with respect to the radius, i.e.:

$$
\Phi(r) \propto 1-q\left(\frac{r}{R}\right)^{2}
$$

where $R$ is the radius of the core. This flux shape leads to the calculation of the differential efficiency $W$. For a spherical reactor, the following is obtained (Weisman 1977, p. 419):

$$
\operatorname{div} \vec{W}=-\frac{48 q^{2} F}{4 \pi \Sigma_{t r} \nu \Sigma_{f} R^{7} \rho_{c}\left(1-\frac{6 q}{5}+\frac{3 q^{2}}{7}\right)}
$$

where $F$ is a form factor accounting for the blankets of radial thickness $\Delta R_{\text {blank }}$ :

$$
F=\frac{\int_{r=0}^{r=R} \nu \Sigma_{f} \Phi^{2} d^{3} r}{\int_{r=0}+\Delta R_{\text {blank }}} \nu \Sigma_{f} \Phi^{2} d^{3} r
$$

In this model, $d i v \vec{W}$ is constant whereas in real-life situations, it decreases with distance from the center of the reactor. Bethe and Tait modeled the pressure using a linear state equation with respect to the difference from the threshold energy:

$$
\left\{\begin{array}{l}
p\left(E, \rho_{c}\right)=0 \quad \text { when } E<E_{\text {threshold }} \\
p\left(E, \rho_{c}\right)=(\gamma-1) \rho_{c}\left(E-E_{\text {threshold }}\right) \quad \text { when } E \geq E_{\text {threshold }}
\end{array}\right.
$$

The $\gamma$ constant is equal to 2 in the historical model. It is the ratio of the heat capacities of the gas and solid in the problem.

### 17.23 Subcritical Approach: Reactor Start-Up

(Murray 1954, p. 159)
For a subcritical reactor, the flux level cannot be maintained constant due to leakage or high amounts of capture. The only means of reaching a permanent state is by introducing a neutron source. Let $S$ be an imposed neutron source. The neutron concentration at equilibrium is given by:

$$
n=S \ell\left(1+k_{e f f}+k_{e f f}^{2}+k_{e f f}^{3}+\ldots\right)=\frac{S \ell}{1-k_{e f f}}
$$

In other words, the source must exactly balance the loss of neutrons due to under-multiplication between two generations, i.e. $n\left(1-k_{e f f}\right)$. However, the source emits $S \ell n$ neutrons between two generations, thus $S \ell n=n\left(1-k_{e f f}\right)$. For a $P W R$ start-up, these sources can be of various types. For the first cores, a spontaneous fission source was used, for instance ${ }_{98}^{252} C f$ inserted in the core only for the very first divergence. The primary source pin is composed of only 0.2 mg of ${ }_{98}^{252} \mathrm{Cf}$ which has an intensity of $4.4 \times 10^{8}$ neutrons $/ \mathrm{s}\left(\bar{\nu}_{258}{ }_{98} \mathrm{Cf}=3,7560\right)$ with a neutron emission spectrum (for three energy groups) of:

$$
\chi_{[14 \mathrm{MeV}, 500 \mathrm{keV}]}=0.996 \quad \chi_{[500 \mathrm{keV}, 50 \mathrm{keV}]}=0.003 \quad \chi_{[50 \mathrm{keV}, 0 \mathrm{eV}]}=0.001
$$

This source is located inside a hermetic double-steel shielded cermet to ensure confinement of fission products. The source pin is inserted at the center of the reactor during the first loading and then withdrawn. When the core is irradiated, the $(\gamma, n)$ reactions produced by antimony-beryllium $S b-B e$ sources, also known as secondary sources, are used, with a more thermal spectrum than that of californium:

$$
\chi_{[14 \mathrm{MeV}, 500 \mathrm{keV}]}=0.040 \quad \chi_{[500 \mathrm{keV}, 50 \mathrm{keV}]}=0.940 \quad \chi_{[50 \mathrm{keV}, 0 \mathrm{eV}]}=0.020
$$

The photons required for the reaction come from the irradiated assemblies, with neutron production being proportional to the level of irradiation of the core. The ( $\alpha$, $n$ ) reactions can also be considered at a lesser level. They are produced by the effect of the $\alpha$-radioactivity from heavy nuclei on light nuclei such as oxygen. Therefore, the neutron concentration, and thus the power, may be augmented by increasing the core reactivity (Fig. 17.31).

In reality, inserting a reactivity step instantaneously is not feasible (and for obvious safety reasons, it is not recommended). Instead, a reactivity ramp is inserted by removing the rods at a given velocity for example. The faster the rods are removed, the faster criticality is reached, but it is also reached at a lower neutron level (Fig. 17.32).

Care must be taken to ensure that the reactivity insertion is slow and well controlled in order to avoid "blind" divergence, i.e. the flux detection systemsin this case, the external chambers-can efficiently detect changes in the neutron flux, especially during recalibration phases. For a continuous reactivity insertion, there is no means of detecting when criticality has been reached based on the neutron level plots.

### 17.24 Reactor Stability

(Advances Nuclear Science and Technology Vol. 6, 1972, p. 45; Akcasu et al. 1971, p. 251; Ash 1979; Weaver 1963, 1968)


Fig. 17.31 Subcritical approach for core start-up


Fig. 17.32 Subcritical approach with insertion of a reactivity ramp

We have seen that, owing to feedback effects, reactivity depends on physical reactor parameters such as component temperatures. Certain feedback effects like moderator temperature have higher time constants than others, such as the Doppler effect, due to the establishment of thermal transfer with the coolant. The existence of an oscillating power regime due to feedbacks has been seriously considered, or even a resonant regime without any countermeasures. In the 1950s, Ackroyd et al. analyzed ${ }^{21}$ the stability criteria for such a problem. Let us start from the kinetics equations with the total power of the reactor $P(t)$ and the contribution to power of the ith group of delayed neutrons, $C_{i}(t)$ (it is no longer the precursor concentration if power is used rather than the usual neutron concentration):

$$
\left\{\begin{aligned}
\frac{d P(t)}{d t} & =\frac{\rho-\beta}{\ell} P(t)+\sum_{i=1}^{6} \lambda_{i} C_{i}(t) \\
\frac{d C_{i}(t)}{d t} & =\frac{\beta_{i} P(t)}{\ell}-\lambda_{i} C_{i}(t)
\end{aligned}\right.
$$

If relatively slow phenomena are considered, i.e. those for which $d P(t) /$ $d t \ll \beta P(t) / \ell$, the term $d P(t) / d t$ can be disregarded without assuming that power is constant. Setting the reduced variables $p(t)=\beta P(t) / \ell$ and $R(t)=\rho(t) / \beta$, the kinetics equations are written as:

$$
\left\{\begin{array}{l}
p(t)(1-R(t))=\sum_{i=1}^{6} \lambda_{i} C_{i}(t) \\
\frac{d C_{i}(t)}{d t}+\lambda_{i} C_{i}(t)=\frac{\beta_{i} p(t)}{\beta}
\end{array}\right.
$$

Using the Nordheim technique, the time variation of the parameters is expressed using an exponential form:

$$
p(t)=p_{0} e^{\omega t} \text { and } C_{i}(t)=C_{i}^{0} e^{\omega t}
$$

This leads to the Nordheim equation with the following notations:

$$
R=1-\sum_{i=1}^{6} \frac{\lambda_{i}}{\omega+\lambda_{i}} \frac{\beta_{i}}{\beta}=\sum_{i=1}^{6} \frac{\omega}{\omega+\lambda_{i}} \frac{\beta_{i}}{\beta}
$$

As previously seen, if $R>0$, the frequency $\omega$ is positive and the power grows exponentially. If $R<0$, all the frequencies are negative and the power decays exponentially. If $R=0$, the power remains stable. If a periodic solution is sought,

[^354]the frequency should be written in the imaginary form $i \omega$ such that $e^{i \omega t}$ is periodic, thus:
$$
R(i \omega)=\sum_{i=1}^{6} \frac{i \omega}{\lambda_{i}+i \omega} \frac{\beta_{i}}{\beta}
$$
$R(i \omega)$ is the characteristic transfer function of the response of the reactor to periodic reactivity insertion.

Reactivity may be expressed in the following form:

$$
\rho(t)=\rho_{\text {control }}(t)+\frac{\partial \rho}{\partial T_{k}}\left(T_{k}-T_{k}^{r e f}\right)
$$

where $\rho_{\text {control }}(t)$ is the reactivity of the control management systems (boron, control rods) with respect to a reference situation and $\partial \rho / \partial T_{k}$ is the differential reactivity coefficient with respect to the $k$ component temperature, compared to a reference temperature $T_{k}^{r e f}$. If the reactivity oscillation effect $\delta \rho=\beta \chi e^{i \omega t}$ is modeled with perturbations:

$$
\left\{\begin{array}{l}
R(t)=R_{0}+r e^{i \omega t} \\
p(t)=p_{0}+\pi e^{i \omega t} \\
C_{i}(t)=C_{i}^{0}+c_{i} e^{i \omega t}
\end{array}\right.
$$

Inserting these formulae in the reduced Nordheim equation and keeping only the first-order terms leads to:

$$
\left\{\begin{array}{l}
\pi+p_{0} r=\sum_{i=1}^{6} \lambda_{i} c_{i} \\
\frac{d c_{i}}{d t}+\lambda_{i} c_{i}=\frac{\beta_{i}}{\beta} \pi
\end{array}\right.
$$

or even:
Nordheim equation perturbed at the first order:

$$
\begin{equation*}
\frac{\pi}{p_{0}}\left(\sum_{i=1}^{6} \frac{i \omega}{\lambda_{i}+i \omega} \frac{\beta_{i}}{\beta}\right)=r \tag{17.29}
\end{equation*}
$$

The oscillation in reactivity creates an oscillation in the temperatures of the materials at the same frequency, but a phase shift for each physical phenomenon (e.g. conduction, convection, etc.) and with a complex transfer function $G_{k}(\omega)$ :

$$
T_{k}(t)=T_{k}^{0}+\frac{\pi}{p_{0}} \beta G_{k}(\omega) e^{i \omega t}
$$

The changes in reactivity and in the feedback parameters can be linked by:

$$
r e^{i \omega t}=\chi e^{i \omega t}+\sum_{k} \frac{\pi}{p_{0}} \alpha_{k} G_{k}(\omega) e^{i \omega t}
$$

where substituting $r$ in Eq. (17.25) gives:

$$
\frac{\pi}{p_{0}}\left(\sum_{i=1}^{6} \frac{i \omega}{\lambda_{i}+i \omega} \frac{\beta_{i}}{\beta}\right)=\chi+\sum_{k} \frac{\pi}{p_{0}} \alpha_{k} G_{k}(\omega)
$$

or: $\frac{\pi}{\chi p_{0}}=\frac{1}{\left(R(i \omega)-\sum_{k} \alpha_{k} G_{k}(\omega)\right)}$
This equation relates the amplitude of the change in power to that of the change in reactivity. The transfer function $R(i \omega)$ may be measured using an oscillation experiment at low power. A resonance phenomenon is possible if $R(i \omega)=\sum_{k} \alpha_{k} G_{k}(\omega)$, which enables the resonant frequency of $\omega_{R}$ to be found. If the latter exists for a power level $p_{0}$ that is lower than the maximum power inducing an emergency stop, the risk of an oscillating resonant amplitude must be considered. It should be noted, however, that the calculations were performed based on the hypothesis that $d P / d t$ is negligible, which is not consistent with resonant behavior. However, the conclusion remains valid as the resonant condition is approached. Stability analysis is of the utmost importance for fast-neutron reactors in which feedback effects are very significant due to their geometry, and for boiling water reactors due to void fraction feedback.

### 17.25 Space-Time Xenon Oscillations

We have seen that the isotope ${ }_{54}^{135} \mathrm{Xe}$ is a highly absorbing fission product. An increase in flux in a region of the core (e.g. by moving the control rods) is associated with a short-term decrease in the ${ }_{54}^{135} \mathrm{Xe}$ concentration (increase in captures), which is compensated by an increase in creation by fission (the medium is more reactive), leading to a decrease in flux due to absorptions being more favorable (Lamarsh and Baratta 2001, p. 383). This effect, stabilizing in theory, is impacted by the delayed effect of ${ }_{53}^{135} \mathrm{I}$, which produces ${ }_{54}^{135} \mathrm{Xe}$ with a 6.61 -hour period. In more detrimental cases, a spatial xenon oscillation is noted in the core and must be the damped by the operator (Weaver 1964, p. 350; Kerkar and Paulin 2008, p. 243). The initial cause of the flux deformation may be the insertion of a control rod, for instance,
which creates an axial oscillation. The equations governing this phenomenon are written (with one energy group) as follows:

$$
\left\{\begin{array}{l}
\frac{d\left[\begin{array}{c}
135 \\
53
\end{array}\right]}{d t}=\gamma_{I} \Sigma_{f} \Phi-\lambda_{I}\left[\begin{array}{c}
{[135} \\
53
\end{array}\right]  \tag{17.30}\\
\frac{d\left[{ }_{54}^{135} X e\right]}{d t}=\gamma_{X e} \Sigma_{f} \Phi+\lambda_{I}\left[{ }_{[ }^{135} I\right]-\lambda_{X e}\left[{ }_{53}^{135} X e\right]-\sigma_{X e} \Phi\left[{ }_{54}^{135} \mathrm{Xe} \mathrm{Xe}\right] \\
\frac{1}{v} \frac{\partial \Phi}{\partial t}-\operatorname{div}(D \overrightarrow{\operatorname{grad}} \Phi)+\Sigma_{a} \Phi=\nu \Sigma_{f} \Phi
\end{array}\right.
$$

Given the xenon time constants, the delayed neutron effect is disregarded. The stationary state is defined by a space-dependent state vector, $u_{0}(\vec{r})=\left(\left[{ }_{53}^{135} I\right]_{0}, \quad\left[{ }_{54}^{135} \mathrm{Xe}\right]_{0}, \Phi_{0}\right)$, and the foregoing system of differential equations may be summarized as:

$$
\frac{\partial u(\vec{r}, t)}{\partial t}=f(u(\vec{r}, t))
$$

$f(u(\vec{r}), t)$ is a non-linear function in $u(\vec{r}, t)$. The stationary state is stable if a perturbation $\Delta u(\vec{r}, t)$ of stationary state $u_{0}(\vec{r})$ tends to zero as time tends to infinity.

$$
\begin{aligned}
\frac{\partial\left(u_{0}(\vec{r})+\delta u(\vec{r}, t)\right)}{\partial t} & =\frac{\partial(\delta u(\vec{r}, t))}{\partial t}=f\left(u_{0}(\vec{r})+\delta u(\vec{r}, t)\right) \\
& \approx \underbrace{f\left(u_{0}(\vec{r})\right)}_{0}+\delta u(\vec{r}, t) \frac{\partial f}{\partial u}\left[u_{0}(\vec{r})\right]
\end{aligned}
$$

In practice, power is linked to changes in isotope temperatures and concentrations via the feedback parameters. Inserting the first-order perturbations $\delta u$ in the state parameters leads to:

$$
\begin{align*}
\delta P & =P-P_{0} \\
& =\alpha_{\text {Doppler }} \underbrace{\left(T^{\text {fuel }}-T_{0}^{\text {fuel }}\right)}_{\delta T^{\text {fuel }}}+\alpha_{\text {Moderator }} \underbrace{\left(T^{\mathrm{mod}}-T_{0}^{\mathrm{mod}}\right)}_{\delta T^{\bmod }}+\ldots=\sum_{\begin{array}{c}
\text { feedback } \\
\text { paramters }
\end{array}} \alpha_{k} \delta u_{k} \tag{17.31}
\end{align*}
$$

Since power is related to the flux by $P=\kappa \Sigma_{f} \Phi$, Eq. (17.26) may be written in the form:

$$
\left\{\begin{array}{l}
\frac{d\left(\left[{ }_{53}^{135} I\right]_{0}+\delta I\right)}{d t}=\gamma_{l} \frac{P_{0}+\delta P}{\kappa}-\lambda_{l}\left(\left[{ }_{53}^{135}\right]_{0}+\delta I\right) \\
\frac{d\left(\left[{ }_{54}^{135 X e}\right]_{0}+\delta X e\right)}{d t}=\gamma_{X e} \frac{P_{0}+\delta P}{\kappa}+\lambda_{l}\left(\left[{ }_{53}^{135 I}\right]_{0}+\delta I\right)-\lambda_{X e}\left(\left[{ }_{54}^{135} X e\right]_{0}+\delta X e\right)-\sigma_{X e} \Phi\left(\left[{ }_{54}^{135} X e\right]_{0}+\delta X e\right) \\
\frac{1 \partial\left(P_{0}+\delta P\right)}{v t}-D \Delta\left(P_{0}+\delta P\right)+\Sigma_{a}\left(P_{0}+\delta P\right)=\nu \Sigma_{f}\left(P_{0}+\delta P\right)
\end{array}\right.
$$

This equation is here synonymous with the fact that the reference state vector $\left(P_{0}, \quad\left[{ }_{53}^{135} I\right]_{0},\left[{ }_{54}^{135} \mathrm{Xe}\right]_{0}, T_{0}^{\text {fuel }}, T_{0}^{\text {mod }}, \ldots.\right)$ verifies Eq. (17.26). Thus, the following system of differential equations for the perturbations is obtained:

$$
\left\{\begin{array}{l}
\frac{d(\delta I)}{d t}=\gamma_{I} \frac{\delta P}{\kappa}-\lambda_{I}(\delta I) \\
\frac{d(\delta X e)}{d t}=\gamma_{X e} \frac{\delta P}{\kappa}+\lambda_{I}(\delta I)-\lambda_{X e}(\delta X e)-\sigma_{X e} \Phi(\delta X e) \\
\frac{1}{v} \frac{\partial(\delta P)}{\partial t}-D \Delta(\delta P)+\Sigma_{a}(\delta P)=\nu \Sigma_{f}(\delta P)
\end{array}\right.
$$

The Laplace operator for the power perturbation may be modeled by a discretization with finite differences for example. Therefore, the values of the perturbations are known at the points surrounding the current point in the spatial mesh. Given that the power perturbation verifies Eq. (17.27), perturbations are generally sought in the following form (Hitchcock 1960):

$$
\frac{d\left(\delta u_{i}\right)}{d t}=\sum_{j=1}^{n} a_{i j} \delta u_{j}
$$

The integer $n$ represents the number of state parameters. Each perturbation is a solution of this system of differential equations of order $n$, and is written as:

$$
\delta u_{j}(\vec{r}, t)=\sum_{i=1}^{n} \delta u_{i j}(\vec{r}) e^{\omega_{j} t}
$$

Hence the non-trivial solution with coefficients $a_{i j}$ verifying the following must be found:

$$
\left|\begin{array}{cccc}
a_{11}-\omega & a_{12} & \cdots & a_{1 n} \\
\vdots & a_{22}-\omega & & \vdots \\
\vdots & & & \vdots \\
a_{n 1} & a_{n 2} & \cdots & a_{n n}-\omega
\end{array}\right|=0
$$

This $n$-degree determinant has $n$ roots $\omega_{j}$, real or complex. Since $\omega$ intervenes only in the form of $a_{j j}-\omega$ on the diagonal, then, if $\omega_{j}=\lambda+i \theta$ is a solution, then so
too will be the complex conjugate $\overline{\omega_{j}}=\lambda-i \theta$. In this case, the stability is guaranteed if all the eigenvalues (frequencies) have a negative real part (Planchard 1995). If only one root is positive or zero, the system is unstable. It can be proved that the imaginary parts are bounded by a constant depending on the physical data of the problem. If the function $u(\vec{r}, t)$ depends on control parameter $c$ (for instance, the absorption of control rods), then change in this parameter beyond a critical value $c_{0}$ may turn the real part of the frequency $\omega_{0} \neq 0$ positive, as a result of which the problem becomes unstable and adopts a stable periodic behavior. This is known as the Hopf bifurcation (1942) (Iooss and Joseph 1995; Callier and Desoer 1991; Merriam 1964).

The increase in the control command parameter beyond $c_{0}$ up to a value of $c_{1}$ may lead to a second frequency $\omega_{1} \neq 0$ (Planchard 1995). Hence, the numerical calculation of the largest eigenvalue for the linearized equations (Eq. 17.27) of a reactor would enable the stability margin to be determined with respect to the action of an operator (insertion/extraction of a control rod). This knowledge optimizes the countermeasures in the event of oscillations. The physics of Fig. 17.33 is as follows: a control rod is inserted in the core (e.g. to lower the power using a rod bank). The immediate decrease in flux and power in the upper part of the core due to absorptions by the rod has two consequences: first, the amount of xenon-135 increases in the upper part since it no longer disappears through captures, and second, the iodine- 135 produced directly by fission-unlike xenon-135, which is formed by the decay of iodine-135-decreases with the flux. This decrease lowers the amount of xenon with a delay due to the decay of iodine $(6.61 \mathrm{~h})$. There is thus a phase difference between the iodine-135 and xenon-135 concentrations, which may remain and lead to an axial-offset power transient of apparent period of $20-30 \mathrm{~h}$, depending on the initial iodine concentration. This phenomenon can lead to an automatic shutdown if the axial-offset power is too positive (power/axial-offset diagram). In practice, the operator may use the regulating bank $R$ to damp the oscillation by inserting the rod bank when power increases in the upper part, and withdrawing it when the sinusoidal function decreases. Experimentally, the phenomenon worsens and becomes more unstable as the core is depleted. In cyclestretching cases with reduced power, the situation worsens as boron is depleted, and the operator may add more boric acid to limit the effluents.

The example illustrated in Fig. 17.34 consists in inserting group $R$ from an all-out (all rods withdrawn) position to that in which 50 steps are still extracted, in 150 s . The rod is left inserted in the core for half an hour and then removed. The effect is observed over a transient lasting 120 h . The xenon- 135 oscillations (the star with eight vertices) and iodine-135 (the star with four vertices) have an amplitude which depends on the power level of the core. Further, these amplitudes are more significant at EOL than at BOL. In addition, the amplitudes may be divergent towards the EOL, thereby indicating that a Hopf bifurcation has been crossed during depletion without any rod problems. These studies also show the existence of a "natural" bifurcation of the reactor during depletion. The axial-offset (star with five vertices) is more prominent when iodine and xenon are out of phase. It should


Fig. 17.33 Xenon oscillation via Hopf bifurcation


Fig. 17.34 Xenon instabilities (studies by Patrick Erhard, EDF, 2008)
be pointed out that the unstable reactor behavior related to a Hopf bifurcation is also characteristic of $B W R$, which tend to become more unstable at low-flow regimes and at high power levels due to void fraction oscillations (incidental transient from LaSalle Reactor, Unit 2 in the USA). ${ }^{22}$

### 17.26 Mechanical Kinetic Effects

We saw previously how changes in thermal-hydraulic parameters influence reactor kinetics. The effect of a geometry variation due to mechanical stresses can also be investigated. A further equation is added to account for the resistance due to inertial acceleration, mechanical damping and elastic resistance to distortions. ${ }^{23}$ The period of mechanical oscillation is assumed to be negligible compared to the mean neutron lifetime including the delayed neutrons (about 10 s ). If $y$ is the (dimensionless) perturbation on the density of material inside the core, it is assumed to obey the following equation:

[^355]$$
\frac{d^{2} y}{d t^{2}}+c_{m} \frac{d y}{d t}+\omega_{m}^{2}(y+b T)=0
$$
where $c_{m}$ is the damping factor, $\omega_{m}$ is the natural mechanical frequency of the component which creates the vibration leading to the change in reactivity, and $b$ the thermal expansion coefficient of the component of mass $M$. This equation is added to the usual equations ( $\alpha_{T}>0$ ):
\[

\left\{$$
\begin{array}{l}
\rho=\rho_{0}-\alpha_{T} T+\alpha_{y} y \\
\frac{d P}{d t}=\frac{\left(-\alpha_{T} T+\alpha_{y} y-\beta+\rho_{0}\right) P+\beta P_{0}}{\ell} \\
P-P_{0}=c_{p} M \frac{d T}{d t}
\end{array}
$$\right.
\]

The temperature is eliminated from the previous equation system, and the following is obtained:

$$
\frac{d^{2} \log \left(\frac{P}{P_{0}}\right)}{d t^{2}}+\frac{\beta}{\ell} \frac{d\left(\frac{P-P_{0}}{P}\right)}{d t}+\frac{\alpha_{T} P_{0}}{c_{p} M \ell}\left(\frac{P-P_{0}}{P}\right)=\frac{\alpha_{y}}{\ell} \frac{d y}{d t}
$$

If the mechanical equation is inserted in the previous equation, a 4th-degree equation on power is reached, using the dimensionless variables $\bar{p} \equiv \log \left(P / P_{0}\right)$ and $p=\left(P-P_{0}\right) / P$ :

$$
\begin{aligned}
& \frac{d^{4} \bar{p}}{d t^{2}}+c_{m} \frac{d^{3} \bar{p}}{d t^{3}}+\omega_{m}^{2} \frac{d^{2} \bar{p}}{d t^{2}}+\frac{\beta}{\ell}\left[\frac{d^{3} p}{d t^{3}}+c_{m} \frac{d^{2} p}{d t^{2}}+\omega_{m}^{2} \frac{d p}{d t}\right]+\omega_{T}^{2}\left[\frac{d^{2} p}{d t^{2}}+c_{m} \frac{d p}{d t}+\omega_{m}^{2} p\right] \\
& \quad+\omega_{m}^{2} \omega_{y}^{2} p=0
\end{aligned}
$$

with $\omega_{T}^{2}=\alpha_{T} P_{0} /\left(c_{p} M \ell\right)$ and $\omega_{y}^{2}=\alpha_{y} b P_{0} /\left(c_{p} M \ell\right)$. In a reactor, the coefficients are such that the system is stable to mechanical stress. Nevertheless, in some cases, a resonance mode may be excited. A stability condition of the type $P_{0} \alpha_{y} b<c_{p} M \beta c_{m}$ is reached. The latter does not depend on the generation time, demonstrating that there is an increasing risk of permanent oscillations with respect to the initial power.

### 17.27 Neutron Noise

(Pazsit and Pal 2007; Annual review of nuclear science Vol. 2, 1953, p. 145; Stacey 2001, p. 177; Thie 1981; Uhrig 1970; Weaver 1964; Williams 1974; Progress in nuclear energy Vol. 9, 1985; Progress in nuclear energy Vol. 15, 1985; Duquesne et al. 1960, p. 195)

The notion of neutron noise covers two different areas. First, the fact that correlation exists between the neutrons of a fission chain in the chain reaction, and second, that pseudo-periodic change in the properties of the medium (geometry, neutron properties, etc.) leads to a variation of same frequency, which may be detected either by a single detector or by comparing the signals for two detectors in different positions.

### 17.27.1 Noise Concept, Spectral Analysis

(Grivet and Blaquière 1958)
If the power of a stabilized reactor is determined by a detector measuring the reaction rate, experimentally, the count rate fluctuates around a mean value. This mean value may be computed in a deterministic way with high precision. Disregarding the mechanical causes (structural vibrations, ${ }^{24}$ formation of steam bubbles, etc.), this change in the count rate originates from the statistical nature of the fission process-each fission does not produce the same number of neutrons. Hence, a fission releasing four neutrons will generate more energy on average during the subsequent fissions than a fission that releases one neutron only. Following the same reasoning, each neutron produced will not travel the same distance in the reactor and will not have the same lifetime. All these phenomena are known only statistically. The large amount of neutrons in the reactor, as well as the creation and loss of neutrons, is connected by random statistical phenomena, which might suggest that the neutron population follows a Poisson distribution ${ }^{25}$ due to the law of large numbers. However, the events that occur are not independent of one another. This correlation between the father and daughter neutrons in a chain reaction is what causes the divergence from Poisson distribution. ${ }^{26}$

Analysis of neutron fluctuations has very interesting applications (Thie 1981): it is possible to study microscopic fluctuations that occur at any power level but which constitute the only stochastic process at very low power, where they can be detected and analyzed. Moreover, the macroscopic fluctuations caused by changes in reactivity due to several factors may also be studied. Finally, neutron fluctuations may occur in cases of geometry perturbation (e.g. assembly vibration, baffle deformation).

Noises are random stochastic phenomena characterized by statistical properties. Three types of noise are generally observed:

[^356]- non-stationary noise whose properties are always time-dependent. By definition, these noises have no mathematically interesting properties.
- stationary noises whose statistical properties are time-independent. This means that the noise is unchanged statistically by any shift in the time basis.
- ergodic noises (Uhrig 1970, p. 10), which are stationary noises if, for several statistically equivalent readings of the noise, the mean reading for a given time interval (statistical mean) is equivalent to the average in time for the same reading (time average).

A noise is said to be centered if its mean value is zero, and Gaussian if its distribution around a mean value obeys a Maxwell-Gauss law. A noise is called white if all frequencies are present in equal degree. Some useful definitions for the analysis of noise include: the auto-correlation function of a noise $x(t)$, given by:

$$
R_{x, x}(\tau) \equiv \lim _{T \rightarrow+\infty} \frac{1}{2 T} \int_{-T}^{+T} x(t) x(t+\tau) d t
$$

The inter-correlation function is written as:

$$
R_{x, y}(\tau) \equiv \lim _{T \rightarrow+\infty} \frac{1}{2 T} \int_{-T}^{+T} x(t) y(t+\tau) d t
$$

The mean power of a noise of frequency $\omega$ is:

$$
P_{x, x}(\omega) \equiv \lim _{T \rightarrow+\infty} \frac{1}{2 T}\left(\int_{-T}^{+T} x(t) e^{-i \omega t} d t\right)^{2}=\int_{-\infty}^{+\infty} R_{x, x}(\tau) e^{-i \omega \tau} d \tau
$$

which is the Fourier transform of the auto-correlation function. The virtually identical concept of Auto Power Spectral Density is also used (Williams 1974, p. 34):

$$
\operatorname{APSD}_{x, x}(\omega) \equiv \frac{1}{2 \pi} \int_{-\infty}^{+\infty} R_{x, x}(\tau) e^{-i \omega \tau} d \tau
$$

and, as a corollary, the inter-correlation power and spectrum (Cross Power Spectral Density):

$$
P_{x, y}(\omega) \equiv \int_{-\infty}^{+\infty} R_{x, y}(\tau) e^{-i \omega \tau} d \tau \text { and } \operatorname{CPSD}_{x, y}(\omega) \equiv \frac{1}{2 \pi} \int_{-\infty}^{+\infty} R_{x, y}(\tau) e^{-i \omega \tau} d \tau
$$

If a noise $y(t)$ is the result of an amplification of a noise $x(t)$ (respectively attenuated) by a transfer function $F(\omega)$, the signal $y(t)$ is:

$$
y(t)=\int_{-\infty}^{+\infty} f\left(t-t^{\prime}\right) x\left(t^{\prime}\right) d t^{\prime} \text { with: } f(t)=\int_{-\infty}^{+\infty} F(\omega) e^{i \omega t} d \omega
$$

The inter-correlation power is worth:

$$
\begin{aligned}
P_{x, y}(\omega) & =\int_{-\infty}^{+\infty} d \tau e^{-i \omega t} \lim _{T \rightarrow+\infty}\left(\frac{1}{2 T} \int_{-T}^{+T} d t x(t) \int_{-\infty}^{+\infty} f\left(t+\tau-t^{\prime}\right) x\left(t^{\prime}\right) d t^{\prime}\right) \\
& =F(\omega) \int_{-\infty}^{+\infty} d t^{\prime} e^{-i \omega\left(t^{\prime}-t\right)} \lim _{T \rightarrow+\infty}\left(\int_{0}^{T} x(t) x\left(t^{\prime}\right) d t\right)=F(\omega) P_{x, x}(\omega)
\end{aligned}
$$

Similarly: $P_{y, y}(\omega)=[F(\omega)]^{2} P_{x, x}(\omega)$. If the transfer function consists of an attenuation $\gamma$ and a delay $\Delta t$, the inter-correlation between $y(t)$ and $x(t)$ is written as:

$$
\begin{aligned}
R_{x, y}(\tau) & \equiv \lim _{T \rightarrow+\infty} \frac{1}{2 T} \int_{-T}^{+T} x(t) y(t+\tau) d t \\
& =\gamma \lim _{T \rightarrow+\infty} \frac{1}{2 T} \int_{-T}^{+T} x(t) y(t+\tau-\Delta t) d t=\gamma R_{x, x}(\tau-\Delta t)
\end{aligned}
$$

thereby, leading to the power:

$$
P_{x, y}(\omega)=\gamma e^{-i \omega \Delta t} \quad P_{x, x}(\omega)
$$

### 17.27.2 Neutron Correlations

In $1944^{27}$ Richard Feynman, Frederic de Hoffman and H. Saber proposed an elementary theory adapted to prompt neutrons, which shows that the probability

[^357]of detecting a first neutron at time 0 , and a second neutron $t$ with the same ancestor as the first neutron in the chain reaction, is given by:
$$
P(t) d t=\left(C+A e^{-\frac{1-k_{e f f}\left(1-\beta_{e f f}\right)}{\ell_{B_{g}}} t}\right) d t
$$
where $C$ corresponds to the non-correlated background noise, which is the product of the detector efficiency, $\varepsilon$, and the neutron concentration, and $A$ is the amplitude coefficient of the correlated part, which is proportional to the average number of prompt fission neutrons $\bar{\nu}$ and to the ratio:
$$
\frac{k_{p}}{1-k_{p}} \equiv \frac{\left(1-\beta_{e f f}\right) k_{e f f}}{1-\left(1-\beta_{e f f}\right) k_{e f f}}
$$

At low power, ${ }^{28}$ in order for the background noise not to overwhelm the correlated part, fundamental reactor properties such as the $\beta_{\text {eff }}$ may be obtained.

If a given reaction (e.g. fission) produces $\nu$ neutrons and occurs $F$ times (fission rate) per second on average, the power of this neutron source is worth $\nu^{2} F$. Denoting $p(\nu)$ as the probability of a fission releasing $\nu$ neutrons (in physics, $\nu$ is always an integer but the problem is considered from a general mathematical point of view, with a probability density), by definition, the following is obtained:

$$
\int p(\nu) d \nu \equiv 1 \text { and } \int \nu p(\nu) d \nu \equiv \bar{\nu}
$$

If there are $n$ neutrons in a reactor, the number of neutrons undergoing sterile capture or escaping from the reactor per unit time is written as follows (using the conventional notation for cross sections in diffusion theory):

$$
\frac{n}{\ell} \frac{\Sigma_{n, \gamma}+D B^{2}}{\Sigma_{f}+\Sigma_{n, \gamma}+D B^{2}}
$$

This is equivalent to giving a negative production value of -1 to this reaction. At the same time, $F_{0}=\frac{n}{\ell} \frac{\Sigma_{f}}{\Sigma_{f}+\Sigma_{n, \gamma}+D B^{2}}$ fissions occurred per second, of which a proportion $p(\nu)$ will release $\nu$ neutrons, with the loss of the fission neutron.

[^358]A production value $\nu-1$ is attributed to this type of reaction. The power of the fission noise is thus calculated as:

$$
P_{\text {fission }}=\frac{n}{\ell} \frac{1}{\Sigma_{f}+\Sigma_{n, \gamma}+D B^{2}}[\left(\Sigma_{n, \gamma}+D B^{2}\right)(-1)^{2}+\Sigma_{f} \underbrace{\int p(\nu)(\nu-1)^{2} d \nu}_{\overline{\nu^{2}}-2 \overline{\bar{v}+1}}]
$$

The criticality condition is written as: $\bar{\nu} \Sigma_{f}=\Sigma_{f}+\Sigma_{n, \gamma}+D B^{2}$, hence:

$$
P_{\text {fission }}=\frac{\frac{n}{\ell} \overline{\nu(\nu-1)}}{\bar{\nu}}=\frac{n}{\ell}\left(\frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}}\right)
$$

If a small reactivity variation of $\rho$ is inserted by disregarding the effect of delayed neutrons, the point-kinetics equations show that the change induced in the amount of neutrons is:

$$
\frac{d n}{d t} \approx \frac{\rho}{\ell} n
$$

This neutron source produces a noise of power:
$P_{\rho, f i s s i o n}=\frac{1}{F_{0}}\left(\frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}^{2}}\right)$ where $F_{0}$ is the number of fissions per second.
$D \equiv\left(\overline{\nu^{2}}-\bar{\nu}\right) / \bar{\nu}^{2}$ is called the Diven factor (Williams 1974, p. 28). As seen earlier, Eq. (17.1) gives the behavior of prompt neutrons in a reactor without any imposed source, i.e.:

$$
n(t)=n(0) e^{\left(\frac{k_{p}-1}{l_{B_{g}}}\right) t}
$$

where $k_{p} \equiv\left(1-\beta_{\text {eff }}\right) k_{\text {eff }}$ is the multiplication factor of prompt neutrons. The use of such a multiplication factor is equivalent to considering one group of fission neutrons without delayed neutrons. In a sub-critical reactor in which an independent source of $S$ neutrons is inserted, the equation governing the neutron population is:

$$
\frac{d n}{d t}=\frac{\rho-\beta_{e f f}}{\ell} n+S=\frac{k_{p}-1}{\ell_{B_{g}}} n+S=-\alpha n+S
$$

Photo 17.5 Bruno Rossi (Public domain)


The coefficient $\alpha \equiv\left(1-k_{p}\right) / \ell_{B_{g}}=\left(\beta_{\text {eff }}-\rho\right) / \ell$ (Uhrig 1970, p. 51; Williams 1974, p. 37), is called the $\alpha-$ Rossi coefficient after Italian physicist Bruno Rossi, ${ }^{29}$ who proposed the first experiments using the fission neutron correlations in 1944. It is for this reason that these techniques are called Rossi $-\alpha$ and are used in several applications, such as measurement of the effective fraction of delayed neutrons (Photo 17.5). ${ }^{30}$

At low power and disregarding delayed neutrons, the reactor behaves like a Markov system ${ }^{31}$ with a correlation time of $1 / \alpha \approx \ell /(\beta-\rho)$.

[^359]

Andrey Markov (1856-1922) (Public domain)
If a neutron counter with a Poisson response function were available, i.e. with a random count rate averaged over several counts (sufficient in statistical terms) proportional to the mean neutron loss, i.e. the sub-critical permanent regime in fission rate $F$, the number of counts per second measured by the counter during a counting time of $\Delta t$ would be (Fig. 17.35):

$$
\langle c\rangle=\varepsilon F \Delta t
$$

In this formula, $\varepsilon$ is the detector efficiency. Let two neutrons be $n^{A}$ and $n^{B}$, each one leading to a fission at time $t_{0}$. The correlation that a daughter neutron contributing to the count rate at time $t_{1}$ (up to $d t_{1}$ ) is of the same family as the neutron contributing to the count rate at $t_{2}$ (up to $d t_{2}$ ) is determined. If all the neutron pairs are counted at these two times, the pair $\left(n_{1}^{A}, n_{2}^{A}\right)$ is from the same father neutron $n^{A}$ (these are called coupled pairs) while the pair $\left(n_{1}^{A}, n_{2}^{B}\right)$ is released by two different

Fig. 17.35 Correlated fission neutrons

fathers (these are called accidental pairs). The occurrence probability that an accidental pair is the product of the occurrence probability of the two events $\left(n_{1}^{A}\right)$ and $\left(n_{2}^{B}\right)$, thus $\varepsilon F d t_{1} \varepsilon F d t_{2}=\varepsilon^{2} F^{2} d t_{1} d t_{2}$ (Williams 1974, p. 39). The occurrence probability for a coupled pair is the result of four probabilities: the probability of fission during a time interval $d t_{1}$, which is $d t_{1} \mathrm{v} \Sigma_{f}=d t_{1} /(\bar{\nu} \ell)$ where $\bar{\nu}$ is the mean number of neutrons produced by fission. Given that one fission at time $t_{0}$ produces $\nu$ neutrons with probability $p(\nu)$, the neutrons released and belonging to this fission descent will be amplified at time $t_{1}$ by a factor of $e^{-\alpha\left(t_{1}-t\right)}$. They therefore increase to $\nu e^{-\alpha\left(t_{1}-t\right)}$ and their probability of contributing to the count rate during the time interval $d t_{1}$ is $\varepsilon \nu e^{-\alpha\left(t_{1}-t\right)} d t_{1} /(\bar{\nu} \ell)$. Following the same reasoning, the probability of another neutron from the same generating fission contributing to the count rate over time $d t_{2}$ is worth $\varepsilon(\nu-1) e^{-\alpha\left(t_{2}-t\right)} d t_{2} /(\bar{\nu} \ell)$. The coefficient $(\nu-1)$ is used due to the fact that the neutron considered is from another fission branch than the first detected neutron, and hence absorbed at $t_{1}$. For a number of fissions $F d t$, the occurrence probability of a coupled pair is the product of the probabilities:

$$
\frac{F d t}{\bar{\nu}^{2} \ell^{2}} \varepsilon^{2} \nu(\nu-1) p(\nu) e^{-\alpha\left(t_{1}+t_{2}-2 t\right)} d t_{1} d t_{2}
$$

The total number of coupled pairs is obtained by integrating over the initial time of the generating fission and over all neutrons produced:

$$
\begin{aligned}
& \int_{-\infty}^{t_{1}} d t \frac{F}{\bar{\nu}^{2} \ell^{2}} \varepsilon^{2} e^{-\alpha\left(t_{1}+t_{2}-2 t\right)} d t_{1} d t_{2} \int_{\nu} d \nu \nu(\nu-1) p(\nu) \\
& \quad=\frac{F}{2 \alpha \bar{\nu}^{2} \ell^{2}} \varepsilon^{2}\left(\overline{\nu^{2}}-\bar{\nu}\right) e^{-\alpha\left(t_{2}-t_{1}\right)} d t_{1} d t_{2}
\end{aligned}
$$

Summing the number of coupled and accidental pairs, the total number of neutron pairs contributing at $d t_{1}$ for the first, and at $d t_{2}$ for the others, is:

$$
\left[\frac{F}{2 \alpha \ell^{2}} \varepsilon^{2} \frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}^{2}} e^{-\alpha\left(t_{2}-t_{1}\right)}+\varepsilon^{2} F^{2}\right] d t_{1} d t_{2}
$$

The $\alpha$-Rossi method consists in studying the decay of the neutron families over a time period of the order of magnitude of $1 / \alpha$. This is done by decomposing the time period into time intervals, called time gates, which may or may not be continuous. A neutron counter is placed in the pile. An impulse triggers the channel selector, which measures the probability of a neutron being counted at instant $[t, t+d t]$ after another has been registered at time $t_{1}=0$. The number of pairs is calculated as follows:

$$
n_{\text {pairs }}(t) d t=\left[\frac{F}{2 \alpha \ell^{2}} \varepsilon^{2} \frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}^{2}} e^{-\alpha t}+\varepsilon^{2} F^{2}\right] d t
$$

Developed initially for fast reactors in having a short generation period and in which several father-daughter neutron chains do not usually overlap, this method works very well at low power where the statistical nature predominates and where the detectors are not saturated.

The reduced variance method consists in measuring the average and the standard deviation of a count rate over a time interval $\Delta t$. For this purpose, we integrate the number of pairs for $t_{1} \in\left[0, t_{2}\right]$ and $t_{2} \in[0, \Delta t]$, i.e.:

$$
\begin{aligned}
\int_{0}^{\Delta t} d t_{2} \int_{0}^{t_{2}} d t_{1}\left[\frac{F}{2 \bar{\nu}^{2} \ell^{2}} \varepsilon^{2} e^{-\alpha\left(t_{2}-t_{1}\right)} \int_{\nu} d \nu \nu(\nu-1) p(\nu)\right] & +\int_{0}^{\Delta t} d t_{2} \int_{0}^{t_{2}} d t_{1} \varepsilon^{2} F^{2}= \\
& \frac{F}{2 \alpha^{2} \ell^{2}} \varepsilon^{2} \frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}^{2}}\left(1-\frac{1-e^{-\alpha \Delta t}}{\alpha \Delta t}\right) \Delta t+\varepsilon^{2} F^{2} \frac{(\Delta t)^{2}}{2}
\end{aligned}
$$

If $c$ is the count rate, the total number of pairs can be directly evaluated by counting the mean number of combinations of pairs of $c$ numbers (integer, with possible extension to real numbers), thus $\langle c(c-1) / 2\rangle=\left(\left\langle c^{2}\right\rangle-\langle c\rangle\right) / 2$. By definition of the mean count rate: $\langle c\rangle \equiv \varepsilon F \Delta t$, where:

$$
\frac{\left\langle c^{2}\right\rangle-\langle c\rangle}{2}=\frac{\langle c\rangle^{2}}{2}+\frac{\langle c\rangle}{2} \frac{\varepsilon}{\alpha^{2} \ell^{2}} \frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}^{2}}\left(1-\frac{1-e^{-\alpha \Delta t}}{\alpha \Delta t}\right)
$$

Since $\alpha \equiv\left(\beta_{\text {eff }}-\rho\right) / \ell$, finally ${ }^{32}$ :

$$
\frac{\left\langle c^{2}\right\rangle-\langle c\rangle^{2}}{\langle c\rangle}=1+\frac{\varepsilon}{\left(\beta_{e f f}-\rho\right)^{2}} \frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}^{2}}\left(1-\frac{1-e^{-\alpha \Delta t}}{\alpha \Delta t}\right)
$$

This expression shows the respective role of the Diven factor, the reactivity and the coefficient $\alpha$. For a true Poisson distribution, $\left(\left\langle c^{2}\right\rangle-\langle c\rangle^{2}\right) /\langle c\rangle=1$ would be obtained. The complementary term represents the difference with respect to Poisson distribution. Hence, measurement of the sub-criticality level can be obtained, with a sample application being measurement of the shutdown antireactivity margin [R. Uhrig in Weaver (1964, p. 1) and T. Stern and J. Valat in Weaver (1964, p. 27)].

[^360]
### 17.27.3 The Feynman- $\alpha$ Method

In a Markov chain, the state of a system at the current time determines its evolution without considering its past states. In other words, the process has "no memory". This is the case for a fissile system without delayed neutrons and its evolution over time is characterized by the probability of having $n$ neutrons at time $t$, given that there were $n_{0}$ at time $t_{0}$, i.e. $p\left(n, t / n_{0}, t_{0}\right)$.

Can this probability be characterized more precisely? If the state at an intermediate time $t_{m}$ is considered, by summing over all the possible intermediate states, the following can be written:

Chapman-Kolmogorov Equation:

$$
\begin{equation*}
p\left(n, t / n_{0}, t_{0}\right)=\sum_{\forall m} p\left(n, t / m, t_{m}\right) p\left(m, t_{m} / n_{0}, t_{0}\right) \tag{17.32}
\end{equation*}
$$

This is the Chapman-Kolmogorov Equation. The probability increment for a time increment of $d t$ is defined as:

$$
w_{n, m}(t) d t \equiv p(n, t+d t / n, t)
$$

This is an infinitesimal transition probability. The normalized probabilities $p(n, t+d t / n, t)$ verify:

$$
\forall t \quad \sum_{n} p(n, t+d t / n, t)=1=\sum_{n} w_{n, m}(t) d t
$$

By introducing the probability $w_{n, n}(t)$, the following may be written:

$$
w_{n, n}(t) d t=1-\sum_{m<n} w_{n, m}(t) d t
$$

The Chapman-Kolmogorov equation is then written by substituting $t$ by $t+d t$ and $t_{m}$ by $t$ :

$$
\begin{aligned}
p\left(n, t+d t / n_{0}, t_{0}\right) & =\sum_{\forall m} w_{n, m}(t) d t p\left(m, t / n_{0}, t_{0}\right) \\
& =\sum_{m<n} w_{n, m}(t) d t p\left(m, t / n_{0}, t_{0}\right)+\left(1-\sum_{m<n} w_{n, m}(t) d t\right) p\left(n, t / n_{0}, t_{0}\right)
\end{aligned}
$$

which is expressed in the form of a differential equation called the direct master equation:

Direct master equation:

$$
\begin{equation*}
\frac{d p\left(n, t / n_{0}, t_{0}\right)}{d t}=\sum_{m<n} w_{n, m}(t) p\left(m, t / n_{0}, t_{0}\right)-\left(\sum_{m<n} w_{n, m}(t) d t\right) p\left(n, t / n_{0}, t_{0}\right) \tag{17.33}
\end{equation*}
$$

What has been developed until now is not connected with neutron physics. Describing the counting process of the detector introduces neutron behavior into the concept. Assuming that the counter is located in or around a reactor to measure the neutron flux, it works by producing a response when neutrons are captured by the detecting surface characterized by a detection cross section $\Sigma_{D}$. Each neutron reacting with the detector is called a "stroke", which is the pulse detected by the incremental stroke counter. The processes describing the transition from one state to another one, i.e. the possibility of obtaining $n$ neutrons at time $t+d t$ and $c$ stroke detections integrated over the time interval $[0, t+d t]$ during a sufficiently small time increment for only one interaction, of any type, to take place, may be described as follows:

- There are $n$ neutrons at time $t$ and the inherent source $S$ of the reactor creates a new neutron. The detector does not detect any strokes, as shown by the following scheme:

- There are $n+1$ neutrons at time $t$ and one of the neutrons is captured in the core. The capture cross section of the latter is $\Sigma_{c}$ and the flux in the core is $\Phi \equiv(n+1) \mathrm{v}$ where v is the speed of the neutrons. The detector does not detect any supplementary strokes:

- There are $n+1-\nu$ neutrons at time $t$ and one neutron induces a fission in the core (the fission cross section being $\Sigma_{f}$ ) leading to the release of $\nu$ new fission neutrons with a distribution $\chi(\nu)$ (the mean value being $\bar{\nu}$ ) and the flux in the reactor is $\Phi \equiv(n+1-\nu) \mathrm{v}$. The detector does not detect any strokes:

- There are $n+1$ neutrons at time $t$ and one of the neutrons interacts with the detector. The detector counts a stroke:


For this problem, the direct master equation is:
Direct master equation for a reactor/detector system:

$$
\begin{align*}
\frac{d p\left(n, c, t / n_{0}, 0, t_{0}\right)}{d t}= & S p\left(n-1, c, t / n_{0}, 0, t_{0}\right) \\
& +(n+1) \mathrm{v} \Sigma_{c} p\left(n+1, c, t / n_{0}, 0, t_{0}\right) \\
& +\sum_{\nu}(n+1-\nu) \mathrm{v} \Sigma_{f} \chi(\nu) p\left(n+1-\nu, c, t / n_{0}, 0, t_{0}\right) \\
& +(n+1) \mathrm{v} \Sigma_{D} p\left(n+1, c-1, t / n_{0}, 0, t_{0}\right) \\
& -\left(S+n \mathrm{v} \Sigma_{c}+n \mathrm{v} \Sigma_{f}+n \mathrm{v} \Sigma_{D}\right) p\left(n, c, t / n_{0}, 0, t_{0}\right) \tag{17.34}
\end{align*}
$$

The last term should be interpreted as the probability of obtaining $n$ neutrons and $c$ strokes at time $t+d t$, given that they were already the same at time $t$. This term is negative in the direct master equation.

To study this differential equation that accounts for the changing number of neutrons per fission via the distribution $\chi(\nu)$, the probability-generating functions were introduced historically. They are defined in a general fashion by:

$$
F(x, y, t)=\sum_{n} \sum_{c} P(n, c, t) x^{n} y^{c} \text { and } f(x)=\sum_{\nu} \chi(\nu) x^{\nu}
$$

It should be noted that $F(1,1, t)=\sum_{n} \sum_{c} P(n, c, t)=1$, and similarly, $f(1)=\sum_{\nu} \chi(\nu)=1$

The time dependence at $t_{0}$ has been omitted for the sake of concision. By deriving these functions, some average values may be computed:

$$
\left\{\begin{array}{l}
\frac{\partial F(x, y, t)}{\partial x}=\sum_{n} \sum_{c} P(n, c, t) n x^{n-1} y^{c} \\
\frac{\partial F(x, y, t)}{\partial y}=\sum_{n} \sum_{c} P(n, c, t) x^{n} c y^{c-1} \\
\frac{\partial f(x)}{\partial x}=\sum_{\nu} \chi(\nu) \nu x^{\nu-1}
\end{array}\right.
$$

It should be pointed out that for the particular values $x=y=1$ :

$$
\left\{\begin{array}{l}
\left.\frac{\partial F(x, y, t)}{\partial x}\right|_{x=y=1}=\sum_{n} \sum_{c} P(n, c, t) n \equiv \bar{n} \\
\left.\frac{\partial F(x, y, t)}{\partial y}\right|_{x=y=1}=\sum_{n} \sum_{c} P(n, c, t) c \equiv \bar{c} \\
\left.\frac{\partial f(x)}{\partial x}\right|_{x=y=1}=\sum_{\nu} \chi(\nu) \nu \equiv \bar{\nu}
\end{array}\right.
$$

Applying the same reasoning, the second derivatives lead to the second-order moments:

$$
\left\{\begin{array}{l}
\left.\frac{\partial^{2} F(x, y, t)}{\partial x^{2}}\right|_{x=y=1}=\sum_{n} \sum_{c} P(n, c, t) n(n-1) \equiv \overline{n(n-1)} \\
\left.\frac{\partial^{2} F(x, y, t)}{\partial y^{2}}\right|_{x=y=1}=\sum_{n} \sum_{c} P(n, c, t) c(c-1) \equiv \overline{c(c-1)} \\
\left.\frac{\partial^{2} F(x, y, t)}{\partial x \partial y}\right|_{x=y=1}=\sum_{n} \sum_{c} P(n, c, t) c n \equiv \overline{c n} \\
\left.\frac{\partial^{2} f(x)}{\partial x^{2}}\right|_{x=y=1}=\sum_{\nu} \chi(\nu) \nu(\nu-1) \equiv \overline{\nu(\nu-1)}
\end{array}\right.
$$

The differential equations governing the generating functions may be established by composition of direct master equations:

$$
\begin{aligned}
\frac{d \sum_{n} \sum_{c} p(n, c, t) x^{n} y^{c}}{d t}= & S \sum_{n} \sum_{c} p(n-1, c, t) x^{n} y^{c} \\
& +\sum_{n} \sum_{c}(n+1) \mathrm{v} \Sigma_{c} p(n+1, c, t) x^{n} y^{c} \\
& +\sum_{n} \sum_{c} \sum_{\nu}(n+1-\nu) \vee \Sigma_{f} \chi(\nu) p(n+1-\nu, c, t) x^{n} y^{c} \\
& +\sum_{n} \sum_{c}(n+1) \mathrm{v} \Sigma_{D} p(n+1, c-1, t) x^{n} y^{c} \\
& -\sum_{n} \sum_{c}\left(S+n \mathrm{v} \Sigma_{c}+n \mathrm{v} \Sigma_{f}+n \mathrm{v} \Sigma_{D}\right) p(n, c, t) x^{n} y^{c}
\end{aligned}
$$

which is written by assuming that $n$ and $c$ are very large, such that

$$
\begin{aligned}
F(x, y, t) & =\sum_{n} \sum_{c} P(n, c, t) x^{n} y^{c} \approx \sum_{n} \sum_{c} P(n-1, c, t) x^{n-1} y^{c} \\
& \approx \sum_{n} \sum_{c} P(n+1, c, t) x^{n+1} y^{c}
\end{aligned}
$$

Similarly: $F(x, y, t)=\sum_{n} \sum_{c} P(n, c, t) x^{n} y^{c} \approx \sum_{n} \sum_{c} P(n, c-1, t) x^{n} y^{c-1}$

Thus, the following equation is reached:

$$
\begin{aligned}
\frac{\partial F(x, y, t)}{\partial t}= & S x \sum_{n} \sum_{c} p(n-1, c, t) x^{n-1} y^{c} p(n-1, c, t) \\
& +\mathrm{v} \Sigma_{c} \sum_{n} \sum_{c}(n+1) p(n+1, c, t) x^{n} y^{c} \\
& +\sum_{n} \sum_{c} \sum_{\nu}(n+1-\nu) \mathrm{v} \Sigma_{f} \chi(\nu) p(n+1-\nu, c, t) x^{n} y^{c} \\
& +\mathrm{v} \Sigma_{D} \sum_{n} \sum_{c}(n+1) p(n+1, c-1, t) x^{n} y^{c} \\
& -\sum_{n} \sum_{c} S p(n, c, t) x^{n} y^{c}+x\left(\sum_{n} \sum_{c} n \mathrm{v} \Sigma_{c}+n \mathrm{v} \Sigma_{f}+n \mathrm{v} \Sigma_{D}\right) p(n, c, t) x^{n-1} y^{c}
\end{aligned}
$$

or:

$$
\begin{align*}
\frac{\partial F(x, y, t)}{\partial t}= & S(x-1) F(x, y, t)+\mathrm{v} \Sigma_{c}(1-x) \frac{\partial F(x, y, t)}{\partial x}+(f(x)-x) \mathrm{v} \Sigma_{f} \frac{\partial F(x, y, t)}{\partial x} \\
& +\mathrm{v} \Sigma_{D}(y-x) \frac{\partial F(x, y, t)}{\partial x} \tag{17.35}
\end{align*}
$$

Deriving this equation with respect to $x$, the following is obtained:

$$
\begin{aligned}
\frac{\partial^{2} F(x, y, t)}{\partial t \partial x} & =S F(x, y, t)-S(x-1) \frac{\partial F(x, y, t)}{\partial x}+\mathrm{v} \Sigma_{c}(1-x) \frac{\partial^{2} F(x, y, t)}{\partial x^{2}} \\
& -\mathrm{v} \Sigma_{c} \frac{\partial F(x, y, t)}{\partial x}+(f(x)-x) \mathrm{v} \Sigma_{f} \frac{\partial^{2} F(x, y, t)}{\partial x^{2}}+\left(\frac{d f(x)}{d x}-1\right) \mathrm{v} \Sigma_{f} \frac{\partial F(x, y, t)}{\partial x} \\
& +\mathrm{v} \Sigma_{D}(y-x) \frac{\partial^{2} F(x, y, t)}{\partial x^{2}}-\mathrm{v} \Sigma_{D} \frac{\partial F(x, y, t)}{\partial x}
\end{aligned}
$$

For the particular case of $x=y=1$, the following is reached:

$$
\frac{d \bar{n}}{d t}=S-\mathrm{v} \Sigma_{c} \bar{n}+\mathrm{v}(\bar{\nu}-1) \Sigma_{f} \bar{n}-\mathrm{v} \Sigma_{D} \bar{n}
$$

This equation may be written in the usual kinetics equation form:

$$
\begin{equation*}
\text { Kinetics of mean number of neutrons: } \frac{d \bar{n}}{d t}=-\alpha \bar{n}+S \tag{17.36}
\end{equation*}
$$

with $\alpha=\mathrm{v} \Sigma_{c}-\mathrm{v}(\bar{\nu}-1) \Sigma_{f}+\mathrm{v} \Sigma_{D}$. Using the usual neutron notations:
$k_{\infty} \equiv \frac{\bar{\nu} \Sigma_{f}}{\Sigma_{a}}$, the generation period or the effective lifetime of prompt neutron $\ell \equiv \frac{1}{v \nu \Sigma_{f}}=\frac{\ell_{B_{g}}}{k_{\text {eff }}}$, the reactivity $\rho \equiv \frac{k_{\text {eff }}-1}{k_{\text {eff }}}$, and the absorption cross section of the reactor: $\Sigma_{a} \equiv \Sigma_{c}+\Sigma_{f}+\Sigma_{D}$. It should be noted that this definition assumes that the
detector is placed inside the reactor, which is not very important given that $\Sigma_{D}$ has a low value in general. The following may be expressed:

$$
\begin{aligned}
\alpha & =\mathrm{v} \Sigma_{c}-\mathrm{v}(\bar{\nu}-1) \Sigma_{f}+\mathrm{v} \Sigma_{D}=\mathrm{v}\left(\Sigma_{a}-\bar{\nu} \Sigma_{f}\right)=\mathrm{v} \bar{\nu} \Sigma_{f}\left(\frac{1}{k_{\infty}}-1\right) \\
& =\frac{1}{\ell}\left(\frac{1+M^{2} B_{g}^{2}}{k_{e f f}}-1\right) \approx-\frac{\rho}{\ell}
\end{aligned}
$$

The differential equation giving the number of strokes is obtained by deriving Eq. (17.4) with respect to the number of strokes is obtained by deriving Eq. (17.4) with respect to $y$ :

$$
\begin{aligned}
\frac{\partial^{2} F(x, y, t)}{\partial t \partial y} & =S(x-1) \frac{\partial F(x, y, t)}{\partial y}+\mathrm{v} \Sigma_{D} \frac{\partial F(x, y, t)}{\partial x}+\mathrm{v} \Sigma_{D}(y-x) \frac{\partial^{2} F(x, y, t)}{\partial x \partial y} \\
& +\mathrm{v} \Sigma_{c}(1-x) \frac{\partial^{2} F(x, y, t)}{\partial x \partial y}+(f(x)-x) \mathrm{v} \Sigma_{f} \frac{\partial^{2} F(x, y, t)}{\partial x \partial y}
\end{aligned}
$$

Applying this equation at $x=y=1$ :

$$
\frac{d \bar{c}}{d t}=\mathrm{v} \Sigma_{D} \bar{n}
$$

The efficiency of the detector is introduced as $\varepsilon \equiv \frac{\Sigma_{D}}{\Sigma_{f}}$.
The equations for the second-order moments are obtained by deriving Eq. (17.4) twice with respect to $x$, to $y$, or to $x$ and $y$.

$$
\left\{\begin{array}{l}
\frac{d \overline{n(n-1)}}{d t}=2 S \bar{n}+\mathrm{v} \Sigma_{f} \overline{\nu(\nu-1)} \overline{n c}-2 \alpha \overline{n(n-1)} \\
\frac{d \overline{c(c-1)}}{d t}=2 \mathrm{v} \Sigma_{D} \overline{n c} \\
\frac{d \overline{n c}}{d t}=S \bar{c}+\mathrm{v} \Sigma_{D} \overline{n(n-1)}-\alpha \overline{n c}
\end{array}\right.
$$

The discrepancies in moments are given as:

$$
\left\{\begin{array}{l}
\mu_{n, n} \equiv \overline{n(n-1)}-(\bar{n})^{2} \\
\mu_{c, c} \equiv \overline{c(c-1)}-(\bar{c})^{2} \\
\mu_{n, c} \equiv \overline{n c}-\bar{n} \bar{c}
\end{array}\right.
$$

Inserted in the previous differential equations, the following equations are obtained:

$$
\left\{\begin{aligned}
\frac{d \mu_{n, n}}{d t} & =-\frac{d(\bar{n})^{2}}{d t}+2 S \bar{n}+\mathrm{v} \Sigma_{f} \overline{\nu(\nu-1)} \bar{n}-2 \alpha \mu_{n, n}-2 \alpha(\bar{n})^{2} \\
& =-2 \bar{n} \underbrace{\frac{d(\bar{n})}{d t}}+2 S \bar{n}+\mathrm{v} \Sigma_{f} \overline{\nu(\nu-1)} \bar{n}-2 \alpha \mu_{n, n}-2 \alpha(\bar{n})^{2} \\
\frac{-\alpha \bar{n}+S}{d t} & =-\frac{d(\bar{c})^{2}}{d t}+2 \mathrm{v} \Sigma_{D}\left(\mu_{n, c}+\bar{n} \bar{c}\right)=-2 \bar{c} \mathrm{v} \Sigma_{D} \bar{n}+2 \mathrm{v} \Sigma_{D}\left(\mu_{n, c}+\bar{n} \bar{c}\right)=2 \mathrm{v} \Sigma_{D} \mu_{n, c} \\
\frac{d \mu_{n, c}}{d t} & =-\frac{d(\bar{n} \bar{c})}{d t}+S \bar{c}+\mathrm{v} \Sigma_{D}\left(\mu_{n, n}+(\bar{n})^{2}\right)-\alpha\left(\mu_{n, c}+\bar{n} \bar{c}\right)
\end{aligned}\right.
$$

## After grouping of terms:

$$
\left\{\begin{array}{l}
\frac{d \mu_{n, n}}{d t}=\mathrm{v} \Sigma_{f} \overline{\nu(\nu-1)} \bar{n}-2 \alpha \mu_{n, n} \\
\frac{d \mu_{c, c}}{d t}=2 \mathrm{v} \Sigma_{D} \mu_{n, c} \\
\frac{d \mu_{n, c}}{d t}=\mathrm{v} \Sigma_{D} \mu_{n, n}-\alpha \mu_{n, c}
\end{array}\right.
$$

The initial value conditions of this differential system at the beginning of the count by the detector are:

$$
\mu_{c, c(t=0)}=0 \text { and } \mu_{n, c(t=0)}=0
$$

If the reactor is stabilized (stationary state), the flux and thus the number of neutrons are constant (therefore, $\bar{n}$ is constant), i.e.:

$$
\frac{d \mu_{n, n}}{d t}=0 \text { where } \mu_{n, n}=\frac{\mathrm{v} \Sigma_{f} \overline{\nu(\nu-1)} \bar{n}}{2 \alpha}
$$

By inserting this result in the expression of $\frac{d \mu_{n, c}}{d t}$ and by integration, the following is obtained:

$$
\mu_{n, c}(t)=\frac{\mathrm{v}^{2} \Sigma_{D} \Sigma_{f} \overline{\nu(\nu-1)} \bar{n}}{2 \alpha^{2}}\left(1-e^{-\alpha t}\right)=\frac{\varepsilon \mathrm{v}^{2} \Sigma_{f}^{2} \overline{\nu(\nu-1)} \bar{n}}{2 \alpha^{2}}\left(1-e^{-\alpha t}\right)
$$

Obviously, for a stabilized reactor, when time tends to infinity, $\mu_{n, c}(t)$ tends to a constant that is proportional to the mean number of neutrons in the reactor and the detector efficiency. We can also compute $\mu_{c, c}$ simply by:

$$
\mu_{c, c}(t)=\frac{\mathrm{v}^{3} \Sigma_{D}^{2} \Sigma_{f} \overline{\nu(\nu-1)} \bar{n}}{\alpha^{2}}\left(t-\frac{1-e^{-\alpha t}}{\alpha}\right)=\frac{\varepsilon^{2} \mathrm{v}^{3} \Sigma_{f}^{3} \overline{\nu(\nu-1)} \bar{n}}{\alpha^{2} t}\left(1-\frac{1-e^{-\alpha t}}{\alpha t}\right)
$$

Integration of the average count rate enables calculation $\bar{c}$ of using the fact that $\bar{c}(0)=0$ :

$$
\frac{d \bar{c}}{d t}=\mathrm{v} \Sigma_{D} \bar{n} \Rightarrow \bar{c}(t)=\mathrm{v} \Sigma_{D} \bar{n} t=\varepsilon \mathrm{v} \Sigma_{f} \bar{n} t
$$

$\bar{c}(t)$ may then be introduced in $\mu_{c, c}(t)$ :

$$
\mu_{c, c}(t)=\bar{c}(t) \frac{\varepsilon \mathrm{v}^{2} \Sigma_{f}^{2} \overline{\nu(\nu-1)}}{\alpha^{2}}\left(1-\frac{1-e^{-\alpha t}}{\alpha t}\right)
$$

While working on the Manhattan Project in the 1940s, Richard Feynman computed the ratio of variance to mean count rate:
$\frac{\overline{c^{2}}-(\bar{c})^{2}}{\bar{c}}=\frac{\overline{c(c-1)}-(\bar{c})^{2}}{\bar{c}}+1=\frac{\mu_{c, c}(t)}{\bar{c}}+1=1+\frac{\varepsilon \mathrm{v}^{2} \Sigma_{f}^{2} \overline{\nu(\nu-1)}}{\alpha^{2}}\left(1-\frac{1-e^{-\alpha t}}{\alpha t}\right)$
Using the Diven factor: $D \equiv \frac{\overline{\nu(\nu-1)}}{\bar{\nu} 2}$ :
Feynman- $\alpha$ formula:

$$
\begin{equation*}
\frac{\overline{c^{2}}-(\bar{c})^{2}}{\bar{c}}=1+\frac{\varepsilon \mathrm{v}^{2} \bar{\nu}^{2} \Sigma_{f}^{2} D}{\alpha^{2}}\left(1-\frac{1-e^{-\alpha t}}{\alpha t}\right)=1+\frac{\varepsilon D}{\alpha^{2} \ell^{2}}\left(1-\frac{1-e^{-\alpha t}}{\alpha t}\right) \tag{17.37}
\end{equation*}
$$

The same formula is found as that established in the paragraph on neutron correlations. The fluctuation in count rate allows measurement of coefficient $\alpha$, which is proportional to the reactivity (Photo 17.6).

Photo 17.6 Richard
Feynman (Public domain)


### 17.27.4 Delayed-Neutron Effect

For a subcritical reactor with a source of delayed neutrons, the delayed-neutron equation is written as:

$$
\left\{\begin{array}{l}
\frac{d n}{d t}=\frac{\left(k_{p}-1\right) k_{e f f}}{\ell} n(t)+\sum_{i} \lambda_{i} C_{i} \\
\frac{d C_{i}}{d t}=\frac{\beta_{i}}{\ell} n(t)+\lambda_{i} C_{i} \quad i=1, \ldots, \text { Number of precursors }
\end{array}\right.
$$

If $p\left(n, C_{i}, t\right)$ is the probability of the state of the reactor, i.e. having $n$ neutrons and $C_{i}$ precursors at time $t$, the variance of the neutron population $\sigma_{n, n}^{2}$ is written as:

$$
\sigma_{n, n}^{2}=\sum_{i} \int_{n} p\left(n, C_{i}, t\right) n^{2} d n-\left(\sum_{i} \int_{n} p\left(n, C_{i}, t\right) n d n\right)^{2}=\left\langle n^{2}\right\rangle-\langle n\rangle^{2}
$$

Similarly, the neutron/precursor covariances are:

$$
\left\{\begin{array}{l}
\sigma_{n, i}^{2}=\int_{n} p\left(n, C_{i}, t\right) n C_{i} d n d C_{i}-\left(\int_{n} p\left(n, C_{i}, t\right) n d n\right)\left(\int_{n} p\left(n, C_{i}, t\right) C_{i} d C_{i}\right)=\left\langle n C_{i}\right\rangle-\langle n\rangle\left\langle C_{i}\right\rangle \\
\sigma_{i, j}^{2}=\int_{n} p\left(n, C_{i}, C_{j}, t\right) C_{i} C_{j} d C_{i} d C_{j}-\left(\int_{n} p\left(n, C_{i}, t\right) d C_{i}\right)\left(\int_{n} p\left(n, C_{j}, t\right) C_{j} d C_{j}\right)=\left\langle C_{i} C_{j}\right\rangle-\left\langle C_{j}\right\rangle\left\langle C_{i}\right\rangle
\end{array}\right.
$$

To move ahead, we must introduce a conditional probability, $p\left(\nu, c_{1}, \ldots, c_{6}\right)$, of an absorption inducing the release of $\nu$ prompt neutrons and $c_{i}$ precursors of the species $i$ (in the six-group precursor families hypothesis). This probability is evaluated by considering all the possible reactions. On one hand, the sterile captures without fission are considered as being worth $1-k_{p} / \bar{\nu}$ with $k_{p} / \bar{\nu}$ the number of absorptions with fission. The fissions are decomposed as:
$\frac{k_{p}}{\bar{\nu}} p(\nu)(1-\bar{\nu} \beta)$ emitting $\nu$ prompt neutrons without emission of delayed neutrons $\frac{k_{p}}{\bar{\nu}} p(\nu) \bar{\nu} \beta_{i}(1-f(\nu, i))$ emitting $\nu$ prompt neutrons and a precursor of species $i . f(\nu$,
$i)$ is the probability of the other possible events when the fission has given $\nu$ prompt neutrons and a precursor $i$.
$\frac{k_{p}}{\bar{\nu}} p(\nu) \bar{\nu} \beta_{i} \bar{\nu} \beta_{j / i}(1-g(\nu, i, j))$ emitting $\nu$ prompt neutrons, a precursor of species
$i$ and a precursor of species $j . \beta_{j / i}$ is the fraction of the conditional production of $j$ given that a precursor $i$ was produced. $g(\nu, i, j)$ is the extension of $f(\nu, i)$ to two precursors.

This reasoning is generalized for six (or more) delayed-neutron groups. In fact, during a given fission, only one or, at most, two precursors may be produced, since
ternary or higher fissions are negligible and the known precursors are seldom in the same father-daughter nuclei chain. Further, assuming that there is no correlation between the emission of prompt neutrons and that of precursors, the problem is simplified:

$$
f(\nu, i)=\beta_{i} g(\nu, i, j)=0 \quad \beta_{j / i}=\beta_{j}
$$

Courant and Wallace proposed ${ }^{33}$ a probability-generating function. The general principles are described in (Williams 1974, p. 20):

$$
F\left(x, y_{i}, y_{j}\right)=1-\frac{k_{p}}{\bar{\nu}}+\frac{k_{p}}{\bar{\nu}}\left(\int_{\nu} d \nu p(\nu) x^{\nu}\left[(1-\bar{\nu} \beta)+\sum_{i, j} \bar{\nu} \beta_{i} y_{i}\left(1-\bar{\nu} \beta_{j}\right)+(\bar{\nu})^{2} \beta_{i} \beta_{j} y_{i} y_{j}\right]\right)
$$

set up such that $F(1,1,1)=1$, the derivatives of which are:

$$
\begin{cases}F_{x}=\left.\frac{\partial F\left(x, y_{i}, y_{j}\right)}{\partial x}\right|_{x=y=1}=k_{p} & F_{y_{i}}=\left.\frac{\partial F\left(x, y_{i} y_{j}\right)}{\partial y_{i}}\right|_{x=y=1}=k_{p} \beta_{i} \\ F_{x, x}=\left.\frac{\partial^{2} F\left(x, y_{i}, y_{j}\right)}{\partial x^{2}}\right|_{x=y=1}=k_{p} \frac{\overline{\nu^{2}}-\bar{\nu}}{\bar{\nu}} & F_{x, y_{j}}=\left.\frac{\partial^{2} F\left(x, y_{i}, y_{j}\right)}{\partial x \partial y_{i}}\right|_{x=y=1}=k_{p} \bar{\nu} \beta_{i} \\ F_{y_{i}, y_{j}}=\left.\frac{\partial^{2} F\left(x, y_{i}, y_{j}\right)}{\partial y_{i} \partial y_{j}}\right|_{x=y=1}=k_{p} \bar{\nu} \beta_{i} \beta_{j} & \end{cases}
$$

With these notations, the differential equations on the variances may be written by averaging the kinetics equations. The derivatives of the generating functions appear in these equations, thereby ensuring that the calculations of these variances are possible.

### 17.27.5 Application to Measurement of Void Fraction Instabilities

The neutron noise methods have been used successfully for boiling-water reactors to investigate the propagation of the void fraction in an assembly cluster. Using axial neutron flux measurements, the auto- and inter-correlations of these signals are measured at different heights $z_{1}$ and $z_{2}$. Fluid mechanics equations show that the transport of the void fraction in a section is written as follows, using the usual conventions:

[^361]$$
\frac{\partial \alpha}{\partial t}+C_{k} \frac{\partial \alpha}{\partial z}=S
$$
with the kinematics wave velocity: $C_{k}=V_{g}+\alpha j \frac{\partial C_{0}}{\partial \alpha}+\alpha \frac{\partial V_{g j}}{\partial \alpha}, V_{g j}$ the relative velocity, $j$ the superficial velocity, and $V_{g}=C_{0} j+V_{g j}$ the interface transfer term:
$$
S=\frac{\Gamma_{g}}{\rho_{g}}\left(1-C_{0} \alpha \frac{\rho_{l}-\rho_{g}}{\rho_{l}}\right)
$$

A classical perturbation analysis around a time-averaged value of the quantities appearing in these equations leads to the equations governing the behavior of these perturbations. Using a Fourier spectral analysis in the simple case in which there is no mass transfer between the liquid and gaseous phases ( $\partial \bar{\alpha} / \partial z=0, \delta S$ $=S-\bar{S}=0$ ), the change in the void fraction at position $z_{2}$ is the delayed image of that existing at $z_{1}$ (Fig. 17.36):

$$
\alpha\left(t, z_{2}\right)=\alpha\left(t-\Delta T, z_{1}\right)
$$

thus: $\delta \alpha\left(\omega, z_{2}\right)=e^{-i \omega \Delta T} \delta \alpha\left(\omega, z_{1}\right)$

Fig. 17.36 Measurement of void fraction fluctuation by neutron noise

with: $\Delta T=\int_{z_{1}}^{z_{2}} \frac{d z}{\overline{C_{k}}}$
At high frequencies (above 1 Hz ), it is considered that only four sub-assemblies of the $B W R$ cluster will significantly influence the measurement, thereby leading to fluctuations in the flux under the form resulting from the effects of the four sub-assemblies:

$$
\left\{\begin{array}{l}
\delta \Phi\left(\omega, z_{2}\right)=\mathrm{A} \sum_{k=1}^{4} \delta \alpha_{k}\left(\omega, z_{2}\right)=\mathrm{A} \sum_{k=1}^{4} e^{-i \omega \Delta T} \delta \alpha\left(\omega, z_{1}\right) \\
\delta \Phi\left(\omega, z_{1}\right)=\mathrm{A} \sum_{k=1}^{4} \delta \alpha_{k}\left(\omega, z_{2}\right)
\end{array}\right.
$$

In these expressions, A is a constant value. The powers of the auto- and intercorrelated noise are given by:

$$
\left\{\begin{array}{l}
P_{\Phi}\left(\omega, z_{1}\right)=\mathrm{A} \sum_{k=1}^{4} P\left(\omega, z_{2}\right) \\
P_{\Phi}\left(\omega, z_{1}, z_{2}\right)=\mathrm{A} e^{-i \omega \Delta T} P_{\Phi}\left(\omega, z_{1}\right)
\end{array}\right.
$$

In a more general and, above all, a more realistic case, in which the mass transfer is not zero, corrective terms taking into account the fluctuation in steam production, $\delta \Gamma_{g}$, and in velocity, $\delta C_{k}$, are incorporated:

$$
P_{\Phi}\left(\omega, z_{1}, z_{2}\right)=\mathrm{A}\left[e^{-i \omega \Delta T} \sum_{k=1}^{4} \gamma_{k} P_{\alpha_{k}}\left(\omega, z_{1}\right)+R(\omega)\right]
$$

Several applications related to random changes in thermal-hydraulic or mechanical conditions are developed in (Williams 1974).

### 17.27.6 Application to Detection of Vibrations

Numerous sources of vibrations impact the reactor core, from the oscillations of structures such as assemblies, the basket supporting the core, and even the vibrations of the primary pumps. ${ }^{34}$ These vibrations modify the neutron flux detected by

[^362]

Fig. 17.37 Oscillation of the basket: the signals in the opposite external chambers are out of phase
the external chambers, which may register signals that are out of phase, as for an oscillation of the basket (Fig. 17.37).

Variations in water gap thickness induce a vibration of the same frequency on the power measurement. The signal spectral analysis ${ }^{35}$ has an enormous amount of data and leads to the detection of unusual signals once the nominal signal is known (Fig. 17.38).

A defect in the integrity of internal structures (e.g. disruption of the flexible support of the thermal shield, fluence of the spacer ring, etc.) is detected by a modification of the vibratory signature. Even the impact of a new fuel (obtained from a new fuel provider) placed at the core periphery has been detected due to the different vibration mode (vibration in $D$ at 3.7 Hz or in $S$ at 6.4 Hz ). Similarly, the presence of baffle water squirts-set up when there is a gap between the baffle

[^363]

Fig. 17.38 Neutron noise measured by the external chambers
plates-has also been detected. Water may force its way through owing to the pressure difference between the by-pass and the active core (head loss between the baffle and the core is different). These squirts may cause breaches in the peripheral pins.

In this way, in August 1985, analysis of neutron noise led to the detection ${ }^{36}$ of a more intense vibration of a rod bank in the Hungarian Paks-2 reactor.

[^364]
# Chapter 18 <br> Computation Methods in Diffusion Theory 

The diffusion equation turns out to be easier to solve than the Boltzmann equation, especially for large 3D reactors. This explains its widespread use in industrial calculation schemes. We will now deal with a few classical methods-without expatiating on the numerical methods used for solving linear systems (there is abundant literature available on this particular subject matter)-so as to focus on the aspects dealing with neutronics.

Hassit in (Progress in nuclear energy Vol. 2, 1958, p. 271; Planchard 1995; Young 1971; Wachspress 1966).

### 18.1 Calculation Meshes

Reactor calculations imply spatial discretization. Using a PWR example, we will consider meshes which are universally used by codes to discretize the diffusion equations and to calculate feedbacks. These meshes take into account the actual borderlines of the constituent elements of the core: the fuel pin assemblies, the supporting grids, the reflectors and the control rods. The physical configuration of a PWR core is represented by a parallelepipedic mesh. Indeed, the assemblies are arranged in a grid and have a square-shaped section. The fuel pins are furthermore arranged in a periodic lattice within an assembly (Figs. 18.1, 18.2, 18.3, and 18.4). Thus, several layers of nested parallelepipedic meshes are employed:

- The neutronic diffusion mesh, normally the most refined mesh, on which the neutron flux is discretized.
- The thermalhydraulics mesh, on which coolant temperatures are discretized.
- The feedback mesh, on which neutron feedback is computed.
- The burn-up mesh, on which fuel burn-up is evaluated.
- The cylindrical thermal mesh (in the case of PWRs), which is used to solve the heat equation for the fuel pin.

Fig. 18.1 Radial geometry of a 900 MWe PWR core


Fig. 18.2 Radial section of a fuel pin


All calculation codes ${ }^{1}$ employ these different meshes to some extent, and some may coincide (e.g. the coolant and feedback meshes). Generally, the different meshes are defined such that one of them "includes" the others to avoid complex mesh projection problems:

- Power, which depends on the flux, is computed on the diffusion mesh.
- All the different thermalhydraulics quantities are defined on the thermalhydraulics mesh.

[^365]Fig. 18.3 Section of the mesh of a set of three assemblies


irradiation mesh


Fig. 18.4 Axial meshes


- Neutronics feedbacks are defined on the feedback mesh. Neutronics quantities such as the cross sections lie on this mesh.
- The burn-up gradients, which show the non-uniform depletion of fuel within a given assembly, are defined on the burn-up mesh. The latter, which takes into account differential fuel burn-up due to variations in feedback parameters, implies that the thermalhydraulics mesh must be equally refined.

For the axial direction, the "inclusion" rules defined above still hold. Nevertheless, the position of supporting grids may be a further constraint if they are modeled by a supplementary absorption term.

### 18.2 Multi-group Diffusion Equations

### 18.2.1 General Case

(Bussac and Reuss 1985; Duderstadt and Hamilton 1976, p. 301; Ferziger and Zweifel 1966, p. 221; Lewis and Miller 1993; Stacey 2001, p. 129; Glasstone and Sesonske 1994, p. 201; Planchard 1995, p. 79; Soodak 1962, p. 119)

Diffusion equations are usually considered using a multi-group approach, that is the energy spectrum range is divided into G intervals or energy groups $\left[E_{g}, E_{g+1}\right]$ for which the multi-group neutron flux $\Phi_{g}$ is computed such that:

$$
\text { Multi-group diffusion equation: } \begin{align*}
& \frac{1}{v_{g}} \frac{\partial \Phi_{g}}{\partial t}-\operatorname{div}\left(D_{g} \overrightarrow{\operatorname{grad}} \Phi_{g}\right)+\Sigma_{t, g} \Phi_{g} \\
= & \chi_{g} \sum_{g^{\prime}=1}^{G} v \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}+\sum_{g^{\prime}=1}^{G} \Sigma_{s, g^{\prime} \rightarrow g} \Phi_{g^{\prime}} \tag{18.1}
\end{align*}
$$

where $\chi_{g}$ is the proportion of neutrons (fast) produced in group $g$. Physical considerations lead to some rules regarding these equations. Above 3 eV , there is no up-scattering (no gain in energy is possible), which leads to a lower limit in energy with separation of the fast flux (where several terms of the slowing-down matrix, which is a triangular matrix, are equivalent to zero) and the thermal flux (where the matrix is full). In practice, the absorption cross section is written in the equation rather than the total cross section, with the presence of the self-scattering term in the RHS term:

$$
\Sigma_{a, g} \Phi_{g}=\Sigma_{t, g} \Phi_{g}-\Sigma_{s, g \rightarrow g} \Phi_{g}
$$

Most industrial PWR codes worldwide use a two-group energy mesh and six delayed neutron groups, the case of Boiling Water Reactors (BWR) generally requires more energy groups to account for strong spectral effects due to axial void fractions. In PWR, the following equations are to be solved:

$$
\left\{\begin{array}{l}
\frac{1}{v_{1}} \frac{\partial \Phi_{1}}{\partial t}=\operatorname{div}\left(D_{1} \overrightarrow{\operatorname{grad}} \Phi_{1}\right)+(1-\beta)\left(v \Sigma_{f, 1} \Phi_{1}+v \Sigma_{f, 2} \Phi_{2}\right)-\left(\Sigma_{a, 1}+\Sigma_{s, 1 \rightarrow 2}\right) \Phi_{1}+\sum_{i=1}^{6} \lambda_{i} C_{i} \\
\frac{1}{v_{2}} \frac{\partial \Phi_{2}}{\partial t}=\operatorname{div}\left(D_{2} \overrightarrow{\operatorname{grad}} \Phi_{2}\right)-\Sigma_{a, 2} \Phi_{2}+\Sigma_{s, 1 \rightarrow 2} \Phi_{1} \\
\frac{\partial C_{i}}{\partial t}=-\lambda_{i} C_{i}+\beta_{i}\left(v \Sigma_{f, 1} \Phi_{1}+v \Sigma_{f, 2} \Phi_{2}\right) \quad \text { for } i=1,6
\end{array}\right.
$$

In a stationary system, the six-group precursor concentrations are given by:

$$
\lambda_{i} C_{i}=\beta_{i}\left(v \Sigma_{f, 1} \Phi_{1}+v \Sigma_{f, 2} \Phi_{2}\right) \quad \text { for } i=1,6
$$

To compute a critical state, an iterative method is used in which the production term is divided by $k_{\text {eff, }}$, which is updated after each iteration. The choice of dividing
the production terms by the multiplication factor is arbitrary (another term of the equation, like the slowing-down term for example, could have been divided), but it appears that this approach was decided by G. Birkhoff and R. S. Varga in the 50s (Planchard 1995, p. 81).

### 18.2.2 "1.5"-group Diffusion

(Stamm'ler and Abbate 1983, p. 436)
As seen earlier, most industrial thermal core calculation schemes use two energy groups: a fast group and a thermal group. The diffusion equations in static are as follows:

$$
\left\{\begin{array}{l}
-\operatorname{div}\left(D_{1} \overrightarrow{\operatorname{grad}} \Phi_{1}\right)+\Sigma_{t, 1} \Phi_{1}=\frac{\sum_{g^{\prime}=1}^{2} \nu \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}}{k_{e f f}}+\Sigma_{s, 1 \rightarrow 1} \Phi_{1}+\Sigma_{s, 2 \rightarrow 1} \Phi_{2} \\
-\operatorname{div}\left(D_{2} \overrightarrow{\operatorname{grad}} \Phi_{2}\right)+\Sigma_{t, 2} \Phi_{2}=\Sigma_{s, 1 \rightarrow 2} \Phi_{1}+\Sigma_{s, 2 \rightarrow 2} \Phi_{2}
\end{array}\right.
$$

The fast flux equation can be decoupled by simplifying the up-scattering term as follows:

$$
\Sigma_{s, 2 \rightarrow 1} \Phi_{2} \approx\left(\Sigma_{s, 2 \rightarrow 1} \frac{\Phi_{2}}{\Phi_{1}}\right)_{\infty} \Phi_{1}
$$

where $\left(\Sigma_{s, 2 \rightarrow 1} \Phi_{2} / \Phi_{1}\right)_{\infty}$ is the asymptotic value computed in an infinite lattice using a spectral code. This approach, also called 1.5 -group diffusion, is used in the French 3D COCCINELLE code at EDF, as well as in other well-known codes (PRESTO, etc.). This simplification speeds up calculations without significantly affecting their precision.

### 18.2.3 Adjoint Diffusion

(Stacey 2001, p. 481)
If a perturbation $\delta \Sigma$ (given that $\delta \nu \Sigma_{f, g^{\prime}}$ is a perturbation of $\nu \Sigma_{f, g^{\prime}}$ ) of the neutronic properties of a critical reactor, leading to a reactivity perturbation $\delta k_{\text {eff }}$ to obtain a new critical state, the equation of the perturbed flux is as follows:

$$
\begin{aligned}
& -\operatorname{div}\left(\left(D_{g}+\delta D_{g}\right) \overrightarrow{\operatorname{grad}}\left(\Phi_{g}+\delta \Phi_{g}\right)\right)+\left(\Sigma_{t, g}+\delta \Sigma_{t, g}\right)\left(\Phi_{g}+\delta \Phi_{g}\right) \\
& =\chi_{g} \sum_{g^{\prime}=1}^{G} \frac{\left(v \Sigma_{f, g^{\prime}}+\delta \nu \Sigma_{f, g^{\prime}}\right)\left(\Phi_{g^{\prime}}+\delta \Phi_{g^{\prime}}\right)}{k_{e f f}+\delta k_{e f f}}+\sum_{g^{\prime}=1}^{G}\left(\Sigma_{s, g^{\prime} \rightarrow g}+\delta \Sigma_{s, g^{\prime} \rightarrow g}\right)\left(\Phi_{g}+\delta \Phi_{g}\right)
\end{aligned}
$$

By multiplying this equation by $\Phi_{g}^{*}$, for now an arbitrary value that verifies $\Phi_{g}^{*}$ $\left(\overrightarrow{r_{S}}\right)=0$ at the limits of the reactor, then integrating the resulting equation over the
total volume of the reactor and summing over the energy groups afterwards, then, using the fact that $\Phi_{g}$ verifies the non-perturbed equation, thereby canceling the first-order terms, and by substracting the non-perturbed equation from the perturbed equation, the following equation is obtained:

$$
\begin{aligned}
& \int_{V} d^{3} r \sum_{g=1}^{G} \Phi_{g}^{*}\left[\begin{array}{l}
-\operatorname{div}\left(D_{g} \overrightarrow{g r a d}\left(\delta \Phi_{g}\right)\right)-\operatorname{div}\left(\delta D_{g} \overrightarrow{g r a d}\left(\Phi_{g}\right)\right)-\operatorname{div}\left(\delta D_{g} \overrightarrow{g r a d}\left(\delta \Phi_{g}\right)\right) \\
+\Sigma_{t, g} \delta \Phi_{g}+\delta \Sigma_{t, g} \Phi_{g}+\delta \Sigma_{t, g} \delta \Phi_{g}
\end{array}\right] \\
& =\int_{V} d^{3} r \sum_{g=1}^{G} \Phi_{g}^{*}\left[\begin{array}{l}
\chi_{g} \sum_{g^{\prime}=1}^{G} \frac{\left(v \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}+v \Sigma_{f, g^{\prime}} \delta \Phi_{g^{\prime}}+\delta v \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}+\delta v \Sigma_{f, g^{\prime}} \delta \Phi_{g^{\prime}}\right)}{k_{e f f}+\delta k_{e f f}} \\
-\chi_{g} \sum_{g^{\prime}=1}^{G} \frac{v \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}}{k_{e f f}}+\sum_{g^{\prime}=1}^{G}\left(\Sigma_{s, g^{\prime} \rightarrow g} \delta \Phi_{g}+\delta \Sigma_{s, g^{\prime} \rightarrow g} \Phi_{g}+\delta \Sigma_{s, g^{\prime} \rightarrow g} \delta \Phi_{g}\right)
\end{array}\right]
\end{aligned}
$$

This expression may be simplified by ignoring second-order terms such as $\delta \Sigma_{t, g}$ $\delta \Phi_{g}$ and by integrating by parts twice the term:

$$
\begin{aligned}
\int_{V} d^{3} r \Phi_{g}^{*} \operatorname{div}\left(D_{g} \overrightarrow{g r a d}\left(\delta \Phi_{g}\right)\right)= & \underbrace{\int_{V} d^{3} r \operatorname{div}\left(\Phi_{g}^{*} D_{g} \overrightarrow{g r a d}\left(\delta \Phi_{g}\right)\right)}_{\int_{S} d^{2} r \Phi_{g}^{*} D_{g} \overrightarrow{g r a d}\left(\delta \Phi_{g}\right) \cdot \vec{n}} \\
& -\underbrace{\int_{V} d^{3} r D_{g} \overrightarrow{g r a d} \Phi_{g}^{*} \cdot \overrightarrow{\operatorname{grad}}\left(\delta \Phi_{g}\right)}_{\int_{V} d^{3} r \operatorname{div}\left(D_{g} \delta \Phi_{g} \overrightarrow{g r a d} \Phi_{g}^{*}\right)-\int_{V} d^{3} r \delta \Phi_{g} \operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}^{*}\right)}
\end{aligned}
$$

The first term on the RHS is rewritten by using the Ostrogradski theorem. The same is done for the second term of the RHS to produce the following:

$$
\begin{aligned}
\int_{V} d^{3} r \Phi_{g}^{*} \operatorname{div}\left(D_{g} \overrightarrow{g r a d}\left(\delta \Phi_{g}\right)\right)= & \int_{S} d^{2} r \Phi_{g}^{*} D_{g} \overrightarrow{\operatorname{grad}}\left(\delta \Phi_{g}\right) \cdot \vec{n} \\
& -\int_{S} d^{2} r \delta \Phi_{g} D_{g} \overrightarrow{g r a d} \Phi_{g}^{*} \cdot \vec{n}+\int_{V} d^{3} r \delta \Phi_{g} \operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}^{*}\right)
\end{aligned}
$$

If the perturbed flux is equivalent to zero at the surface $S$, as is the non-perturbed flux, then $\delta \Phi_{g}$ is also equivalent to zero, and the second term is thus canceled out. Since $\Phi_{g}^{*}$ was chosen such that it is zero at the boundary, the first term is hence zero also. Now, only the third term remains. By inserting this result in the initial equation, after inverting $g$ and $g^{\prime}$, we obtain the following:

$$
\int_{V} d^{3} r \sum_{g=1}^{G} \delta \Phi_{g}\left[-\operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}^{*}\right)+\Sigma_{t, g} \Phi_{g}^{*}-\frac{v \Sigma_{f, g}}{k_{e f f}+\delta k_{e f f}} \sum_{g^{\prime}=1}^{G} \chi_{g^{\prime}} \Phi_{g^{\prime}}^{*}-\sum_{g^{\prime}=1}^{G} \Sigma_{s, g \rightarrow g^{\prime}} \Phi_{g^{\prime}}^{*}\right]=0
$$

This equation can only be verified for all values of $\delta \Phi_{g}$ if the term between square brackets is zero. This equation is simply the multi-group diffusion equation where the source and slowing-down operators are transposed. In the chapter on the transport equation, we have seen that this corresponds to the adjoint equation, which is found in perturbation theory. Thus, $\Phi_{g}^{*}$ is the multi-group adjoint flux. The reader will note that the boundary condition used for the adjoint flux (equivalent to zero at the surface) does not correspond to the boundary condition used to define the neutronics importance (angular importance equivalent to zero for inwards directions).

In addition, the adjoint flux of the one-group diffusion problem is equal to the direct flux under the same boundary conditions (Duderstadt and Hamilton 1976, p. 222), since the diffusion, absorption and production operators are all self-adjoint at one-energy group.

### 18.2.4 Taking into Account the Neutron Over-Production Cross Sections

It is sometimes needed to take into account uncommon-reaction cross sections ( $\Sigma_{n, 2 n}, \Sigma_{n, 3 n}, \ldots$ ) in the multi-group diffusion equations. This is done by adding loss of neutrons in the left hand side of the equations and adding new production of neutrons on the right hand side, including a multiplicity factor:

$$
\begin{aligned}
& \underbrace{\frac{1}{v_{g}} \frac{\partial \Phi_{g}}{\partial t}}_{\text {time increase }} \underbrace{-\operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}\right)}_{\text {leakage }}+\underbrace{\Sigma_{a, g} \Phi_{g}}_{\text {absorption }}+\underbrace{\left[\Sigma_{n, n^{\prime}, g \rightarrow g}+\Sigma_{n, 2 n^{\prime}, g \rightarrow g}+\Sigma_{n, 3 n^{\prime}, g \rightarrow g}\right] \Phi_{g}}_{\text {loss through inelastic scattering inside the group itself }} \\
& +\underbrace{\sum_{g^{\prime}=g+1}^{G}\left[\Sigma_{n, n^{\prime}, g \rightarrow g^{\prime}}+\Sigma_{n, 2 n^{\prime}, g \rightarrow g^{\prime}}+\Sigma_{n, 3 n^{\prime}, g \rightarrow g^{\prime}}\right] \Phi_{g}}_{\text {loss through inelastic scattering to other groups }}+\underbrace{\sum_{g^{\prime}=g}^{G} \Sigma_{n, n, g \rightarrow g^{\prime}} \Phi_{g}} \\
& \text { loss through elastic scattering } \\
& \text { slowing down to more thermal groups } \\
& =\underbrace{\frac{\chi_{g} \sum_{g^{\prime}=1}^{G} v \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}}{k_{e f f}}}_{\text {production per fission }}+\underbrace{\sum_{g^{\prime}=1}^{g-1}\left[\Sigma_{n, n^{\prime}, g^{\prime} \rightarrow g}+2 \Sigma_{n, 2 n^{\prime}, g^{\prime} \rightarrow g}+3 \Sigma_{n, 3 n^{\prime}, g^{\prime} \rightarrow g}\right] \Phi_{g^{\prime}}}_{\text {arrival hrough inelastic scattering from faster groups }} \\
& +\underbrace{\left[\Sigma_{n, n^{\prime}, g \rightarrow g}+2 \Sigma_{n, 2 n^{\prime}, g \rightarrow g}+3 \Sigma_{n, 3 n^{\prime}, g \rightarrow g}\right] \Phi_{g}}_{\text {arrival through inelasticscattering inside the group itself }}+\underbrace{\sum_{g^{\prime}=1}^{g} \Sigma_{n, n, g^{\prime} \rightarrow g} \Phi_{g^{\prime}}}
\end{aligned}
$$

A simple hypothesis is made that all new neutrons arrive in the same group ( 2 for $\Sigma_{n, 2 n}, 3$ for $\left.\Sigma_{n, 3 n}, \ldots\right)$. If it is not the case, an "appearance" probability should be taken into account similar to a Watt spectrum. Notation $\Sigma_{n, n}$, means inelastic scattering, where $\Sigma_{n, n}$ means elastic scattering. As well for the neutron overproducing cross sections, in most usual discretization of the energy groups, the loss term per elastic scattering simplifies in two terms: first, scattering inside the group itself, and second, scattering in the adjacent inferior group:

$$
\sum_{g^{\prime}=g}^{G} \Sigma_{n, n, g \rightarrow g^{\prime}} \Phi_{g} \approx \Sigma_{n, n, g \rightarrow g} \Phi_{g}+\Sigma_{n, n, g \rightarrow g+1} \Phi_{g}
$$

As well as for the arrival through elastic scattering from faster groups:

$$
\sum_{g^{\prime}=1}^{g} \Sigma_{n, n, g^{\prime} \rightarrow g} \Phi_{g^{\prime}} \approx \Sigma_{n, n, g-1 \rightarrow g} \Phi_{g-1}+\Sigma_{n, n, g \rightarrow g} \Phi_{g}
$$

If should be pointed out that there is no elastic loss through $\Sigma_{n, 2 n, g \rightarrow g^{\prime}}$ as a new free neutron is produced, therefore it is for sure an inelastic reaction. Equations are strongly simplified using:

$$
\Sigma_{s, g}^{\text {elast }} \equiv \sum_{g^{\prime}=g}^{G} \Sigma_{n, n, g \rightarrow g^{\prime}} \text { and } \Sigma_{s, g^{\prime} \rightarrow g}^{\text {inelast }} \equiv \Sigma_{n, n^{\prime}, g^{\prime} \rightarrow g}+2 \Sigma_{n, 2 n^{\prime}, g^{\prime} \rightarrow g}+3 \Sigma_{n, 3 n^{\prime}, g^{\prime} \rightarrow g}+\ldots
$$

### 18.3 The Power Iteration Method

(Gastinel 1966, p. 334; Planchard 1995, p. 129; Stewart 1973, p. 340; Strang and Fix 1973, p. 216; Wachspress 1966, p. 83)

### 18.3.1 General Considerations

Given an operator $K$ with $k_{i}$ eigenvalues, ordered such that $\left|k_{1}\right| \geq\left|k_{2}\right| \geq\left|k_{3}\right| \cdots$, corresponding to the eigenfunctions $\Phi_{i}$ by choosing the normalization $\int \Phi_{i}^{2} d^{3} r$ $=1$ for the eigenfunctions:

$$
K\left[\Phi_{i}\right]=k_{i} \Phi_{i}
$$

Any value of the flux $\Phi$ can be expanded as a linear combination of the eigenfunctions:

$$
\Phi=\sum_{i} \varphi_{i} \Phi_{i}
$$

Applying $K$ successively to the flux, we obtain:

$$
K[\Phi]=\sum_{i} \varphi_{i} k_{i} \Phi_{i}, \quad K^{2}[\Phi] \equiv K[K[\Phi]]=\sum_{i} \varphi_{i} k_{i}^{2} \Phi_{i}, K^{3}[\Phi]=\sum_{i} \varphi_{i} k_{i}^{3} \Phi_{i} \quad \cdots
$$

If $\left|k_{1}\right|>\left|k_{2}\right| \geq\left|k_{3}\right| \cdots$, then $\lim _{n \rightarrow \infty} \frac{1}{k_{1}^{n}} K^{n}[\Phi]=\Phi_{1}$ and $k_{1}=\lim _{n \rightarrow \infty} \frac{K^{n}[\Phi]}{K^{n-1}[\Phi]}$
At any point in the reactor, the limit value of $K^{n}[\Phi] / K^{n-1}[\Phi]$ tends towards the largest eigenvalue. It is possible to determine an algorithm to obtain the second eigenvalue. ${ }^{2}$ We also show that if $\varphi_{1}=0$, the algorithm converges towards the second eigenfunction. Assuming:

$$
\Phi=\sum_{i}\left(\varphi_{i}+x \psi_{i}\right) \Phi_{i}
$$

By applying the $K$ operator $n$ times, and assuming that the eigenvalues are well ordered, we obtain:

$$
\left\{\begin{array}{l}
\lim _{n \rightarrow \infty} \frac{1}{k_{1}^{n}} K^{n}[\Phi]=\lim _{n \rightarrow \infty} \frac{1}{k_{1}^{n}}\left(\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n} \Phi_{1}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n} \Phi_{2}\right) \\
\lim _{n \rightarrow \infty} \frac{K^{n}[\Phi]}{K^{n-1}[\Phi]}=\lim _{n \rightarrow \infty} \frac{\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n} \Phi_{1}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n} \Phi_{2}}{\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n-1} \Phi_{1}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n-1} \Phi_{2}}
\end{array}\right.
$$

The arbitrary choice of $x=-\psi_{1} / \varphi_{1}$ leads to a limit value of $k_{2}$, when the choice $x=-\psi_{2} / \varphi_{2}$ leads to $k_{1}$. Nevertheless, $\varphi_{1}, \psi_{1}, \varphi_{2}, \psi_{2}$ are all unknowns in our problem. Given that the method converges within the reactor, it is sufficient to choose two regions. The scalar product for region $V_{j}$ is defined as:

$$
\langle f, g\rangle_{V_{j}} \equiv \int_{V_{j}} f . g d^{2} r
$$

Whence:
$\lim _{n \rightarrow \infty} \int_{V_{j}}\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n} \Phi_{1}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n} \Phi_{2} d^{3} r=\lim _{n \rightarrow \infty}\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n}\left\langle\Phi_{1}, 1\right\rangle_{V_{j}}+$ $\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n}\left\langle\Phi_{2}, 1\right\rangle_{V_{j}}$ The eigenvalues computed over the two zones $V_{\alpha}$ and $V_{\beta}$ are the same, thus leading to:

[^366]\[

$$
\begin{aligned}
k_{\alpha} & =\lim _{n \rightarrow \infty} \frac{\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n}\left\langle\Phi_{1}, 1\right\rangle_{V_{\alpha}}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n}\left\langle\Phi_{2}, 1\right\rangle_{V_{\alpha}}}{\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n-1}\left\langle\Phi_{1}, 1\right\rangle_{V_{\alpha}}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n-1}\left\langle\Phi_{2}, 1\right\rangle_{V_{\alpha}}} \\
& =\lim _{n \rightarrow \infty} \frac{\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n}\left\langle\Phi_{1}, 1\right\rangle_{V_{\beta}}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n}\left\langle\Phi_{2}, 1\right\rangle_{V_{\beta}}}{\left(\varphi_{1}+x \psi_{1}\right) k_{1}^{n-1}\left\langle\Phi_{1}, 1\right\rangle_{V_{\beta}}+\left(\varphi_{2}+x \psi_{2}\right) k_{2}^{n-1}\left\langle\Phi_{2}, 1\right\rangle_{V_{\beta}}}=k_{\beta}
\end{aligned}
$$
\]

Using $x=-\psi_{1} / \varphi_{1}$ over one region and $x=-\psi_{2} / \varphi_{2}$ over another, it is possible to calculate the two eigenvalues on the fly. The error on $k_{2}$ decays in $\left(\left|k_{3}\right| /\left|k_{2}\right|\right)^{n}$, while the error on $k_{1}$ decays as $\left(\left|k_{3}\right| /\left|k_{1}\right|\right)^{n}$.

### 18.3.2 Matrix Representation

Classically, we may write the equation system in matrix form. For the sake of brevity, we will focus on a system of two equations with two energy groups without any up-scattering, without any loss of generality for the multi-group problem. Given the operators (without up-scattering):

$$
\left\{\begin{array}{l}
A_{1}=-\operatorname{div}\left(D_{1} \overrightarrow{\operatorname{grad}}[]\right)+\Sigma_{a, 1}[]+\Sigma_{1 \rightarrow 2}[] \\
A_{2}=-\operatorname{div}\left(D_{2} \overrightarrow{\operatorname{grad}}[]\right)+\Sigma_{a, 2}[]
\end{array}\right.
$$

We therefore have the following:

$$
\underbrace{\left(\begin{array}{cc}
A_{1} & 0 \\
-\Sigma_{s, 1 \rightarrow 2} & A_{2}
\end{array}\right)}_{A}\left[\begin{array}{l}
\Phi_{1} \\
\Phi_{2}
\end{array}\right]=\frac{1}{k_{e f f}} \underbrace{\left(\begin{array}{cc}
\nu \Sigma_{f, 1} & \nu \Sigma_{f, 2} \\
0 & 0
\end{array}\right)}_{B} \underbrace{\left[\begin{array}{l}
\Phi_{1} \\
\Phi_{2}
\end{array}\right]}_{\Phi}
$$

Which we may write in matrix form with an eigenvalue problem (Durand 1961; Wilkinson 1965):

$$
K[\Phi]=k \Phi
$$

where $K=A^{-1} B$. The production term is artificially and arbitrarily divided by the multiplication factor $k_{\text {eff }}$, transforming the criticality problem to an eigenvalue problem. This mathematical shortcut enables numerical iteration over a given parameter. The physical solution being actually sought to obtain the neutron flux should be positive everywhere. Mathematically, this corresponds to searching the neutron flux for the largest eigenvalue. The flux is determined up to the nearest multiplication factor. The latter is evaluated by normalizing the powers per assembly (which are derived from the neutron flux via the energy production cross section $\kappa \Sigma_{f}$ to the power of the whole core. The system to be solved consists of two coupled equations. The power iteration method (Stacey 2001, p. 84; Duderstadt and

Hamilton 1976, p. 219), potentially accelerated by a semi-iterative Chebychev method (Wachspress 1966, p. 157; Hageman and Young 1981, p. 45), may be used to compute the $k_{\text {eff }}$ and the fast and thermal neutron fluxes. Let the fission source be equal to $\Psi=\nu \Sigma_{f, 1} \Phi_{1}+\nu \Sigma_{f, 2} \Phi_{2}$, giving:

$$
\binom{\Phi_{1}}{\Phi_{2}}=\frac{1}{k_{e f f}}\binom{A_{1}^{-1} \Psi}{A_{2}^{-1} \Sigma_{s, 1 \rightarrow 2} A_{1}^{-1} \Psi}
$$

Applying matrix $B$ to the above system, we obtain:

$$
\begin{aligned}
B \Phi & =\binom{\nu \Sigma_{f, 1} \Phi_{1}+\nu \Sigma_{f, 2} \Phi_{2}}{0} \equiv\binom{\Psi}{0}=\frac{1}{k_{e f f}}\binom{\nu \Sigma_{f, 1} A_{1}^{-1} \Psi+\nu \Sigma_{f, 2} A_{2}^{-1} \Sigma_{1 \rightarrow 2} A_{1}^{-1} \Psi}{0} \\
& \equiv \frac{1}{k_{e f f}} T[\Psi]
\end{aligned}
$$

We are, therefore, led to solve the $T[\Psi]=k_{e f f} \Psi$ system with $T[] \equiv \nu \Sigma_{f, 1} A_{1}^{-1}+$ $\nu \Sigma_{f, 2} A_{2}^{-1} \Sigma_{s, 1 \rightarrow 2} A_{1}^{-1}$. In fact, we are looking for the largest eigenvalue of matrix $T$. We use the power iteration method for this purpose as it allows the search for the largest eigenvalue for a square matrix. Assuming that $\Psi^{n}$ and $k_{e f f}^{n}$ are known for the $n$ external iteration, we can calculate $\Psi^{n}=\nu \Sigma_{f, 1} \Phi_{1}^{n}+\nu \Sigma_{f, 2} \Phi_{2}^{n}$ by solving the following equation system:

$$
\left\{\begin{aligned}
A_{1} \Phi_{1}^{n+1} & =\frac{1}{k_{e f f}^{n}} \Psi^{n} \\
A_{1} \Phi_{2}^{n+1} & =\Sigma_{s, 1 \rightarrow 2} \Phi_{1}^{n+1}
\end{aligned}\right.
$$

When convergence is reached, we obtain: $T\left[\Psi^{n}\right]=k_{e f f} \Psi^{n}$ where: $\Psi^{n+1}=k_{e f f} \Psi^{n} / k_{\text {eff }}^{n}$. This allows the eigenvalue to be updated:

$$
k_{e f f}^{n+1}=\frac{\left\langle\Psi^{n+1} \mid \Psi^{n+1}\right\rangle}{\left\langle\Psi^{n+1} \mid \Psi^{n}\right\rangle} k_{e f f}^{n}
$$

where the scalar product is defined as a volume integral:

$$
\left\langle\Psi^{n+1} \mid \Psi^{n+1}\right\rangle=\int_{\text {reactor }} \Psi^{n+1} \Psi^{n+1} d^{3} r\left\langle\Psi^{n+1} \mid \Psi^{n}\right\rangle=\int_{\text {reactor }} \Psi^{n+1} \Psi^{n} d^{3} r
$$

Convergence can be tested either by the relative variation of $k_{e f f}^{n+1}$ with respect to $k_{\text {eff }}^{n}$, with no guarantee of convergence on the fluxes, or by calculating $\overline{k_{\text {eff }}^{n+1}} \equiv k_{\text {eff }}^{n}$ $\max _{i \in \text { mesh }}\left(\Psi_{i}^{n+1} / \Psi_{i}^{n}\right)$ and $\underline{k_{e f f}^{n+1}} \equiv k_{e f f}^{n} \min _{i \in \text { mesh }}\left(\Psi_{i}^{n+1} / \Psi_{i}^{n}\right)$ to ensure convergence when:

$$
\frac{\overline{k_{\text {eff }}^{n+1}}-\underline{k_{\text {eff }}^{n+1}}}{k_{\text {eff }}^{n+1}} \leq \varepsilon
$$

This last criterion encompasses global convergence on $k_{\text {eff }}$ as well as convergence on the fluxes, with the former converging much faster than the latter. Since the global convergence of the power iteration method is slow, it is usually accelerated using the Chebyshev polynomials. The iterations that calculate $\Phi_{1}^{n+1}$ and $\Phi_{2}^{n+1}$ as a function of $\Phi_{1}^{n}$ and $\Phi_{2}^{n}$ are called inner iterations. They are the iterations that solve the two linear systems.

### 18.3.3 Chebyshev Acceleration

(Planchard 1995, p. 137)
Assuming that the eigenvalue $k_{\text {eff }}$ is known, the solution vector $\Psi$ verifies the following equation (Photo 18.1):

$$
\psi=\frac{1}{k_{e f f}} T \psi \equiv Q \psi, \quad \text { with }: \quad Q \equiv \frac{1}{k_{e f f}} T
$$

If it is further supposed that $k_{\text {eff }}^{n}$ is sufficiently close to $k_{\text {eff }}$ (in practice, this is rapidly the case as the convergence on the eigenvalue is very fast whereas that on the eigenvector requires a larger number of iterations), the error defined by $\varepsilon_{n}=\Psi^{n}$ $-\Psi$ is written as:

Photo 18.1 Pafnuty
Chebyshev (1821-1894)
(Public domain)


$$
\varepsilon_{n}=Q \varepsilon_{n-1}=\underbrace{Q \cdot Q \cdots Q}_{n \text { times }} \varepsilon_{0}=Q^{n} \varepsilon_{0}
$$

where $\varepsilon_{0}$ is the initial error. The goal is to create a polynomial acceleration method. Thus, instead of multiplying the initial error by a power of $Q$, it is multiplied by a polynomial expression in $Q$. The solution obtained by this acceleration method is denoted as $\widetilde{\psi}^{m}$ and $\widetilde{\varepsilon}_{n}=\widetilde{\psi}^{n}-\psi$ the accelerated error at the $n$th iteration. If all the eigenvalues of $Q$ are real and the eigenvectors generate the complete solution space (although positive-definite, the matrix is not symmetric), we can write:

$$
\varepsilon=\sum_{i} \alpha_{i} \varphi_{i} \text { where: } \widetilde{\varepsilon}_{n}=P_{n}(Q) \varepsilon=\sum_{i} \alpha_{i} P_{n}\left(\lambda_{i}\right) \varphi_{i}
$$

where $\lambda_{i}$ and $\varphi_{i}$ are the eigenvalues and eigenvectors of matrix $T$ respectively, with $\lambda_{0}=k_{\text {eff }}$ being the largest eigenvalue and $0<\lambda_{n}<\lambda_{n-1}<\cdots<\lambda_{1}<\lambda_{0}$. Mathematically speaking, the power iteration method exhibits convergence problems as the dominance ratio $P_{m}(x)$ approaches one. Hence, a polynomial acceleration of this type is equivalent to finding polynomials called residual polynomials that verify $P_{m}(1)=1$ and such that $\underbrace{\operatorname{Max}}_{i=1, n}\left\{P_{m}\left(\lambda_{i}\right)\right\}$ is minimal. The Chebyshev polynomials verify this constraint (this property was used earlier in the chapter on the transport equation). They are defined as:

Chebyshev polynomials: $\left\{\begin{array}{l}T_{0}(x)=1 \\ T_{1}(x)=x \\ T_{m+1}(x)=2 x T_{m}(x)-T_{m-1}(x) \quad \text { for } m \geq 2\end{array}\right.$

Analytically, the Chebyshev polynomial $T_{m}(x)$ of degree $m$ is written as:

$$
T_{m}(x)=\left\{\begin{array}{lll}
\cos (m \arccos (x)) & \text { if } & |x|<1 \\
\operatorname{ch}(m \arg \operatorname{ch}(x)) & \text { if } & |x| \geq 1
\end{array}\right.
$$

Here, the appropriate values of $P_{m}(x)$ are given as:

$$
P_{m}(x)=\frac{T_{m}\left(\frac{2}{\sigma} x-1\right)}{T_{m}\left(\frac{2}{\sigma}-1\right)}
$$

A cyclic Chebyshev semi-iteration method consists of partitioning the outer iterations into cycles of Chebyshev iterations. The maximum length of the cycle
is ten outer iterations. The index of the outer iteration is denoted $m+p$ and $p$ is that of the current Chebyshev iteration. The value being sought is $\widetilde{\Psi}^{m+p}$. The recurrence relation describes the evolution of the accelerated errors:

$$
\text { For } p=1 \widetilde{\varepsilon}_{m+1}=P_{1}(Q) \varepsilon_{m}=\frac{T_{1}\left(\frac{2}{\sigma} Q-I\right)}{T_{1}\left(\frac{2}{\sigma}-1\right)} \varepsilon^{m}=\frac{4}{\sigma} \alpha_{1} Q \varepsilon_{m}-2 \alpha_{1} \varepsilon_{m}
$$

For $p>1$, thanks to the recurrence relation on the Chebyshev polynomials:

$$
\begin{aligned}
\widetilde{\mathcal{\varepsilon}}_{m+p} & =P_{p}(Q) \varepsilon_{m}=\frac{T_{p}\left(\frac{2}{\sigma} Q-I\right)}{T_{p}\left(\frac{2}{\sigma}-1\right)} \varepsilon_{m} \\
& =\frac{T_{p-1}\left(\frac{2}{\sigma}-1\right)}{T_{p}\left(\frac{2}{\sigma}-1\right)} 2\left(\frac{2}{\sigma} Q-I\right) \underbrace{P_{p-1}(Q) \varepsilon_{m}}_{\widetilde{\varepsilon}_{m+p-1}}-\frac{T_{p-2}\left(\frac{2}{\sigma}-1\right)}{T_{p}\left(\frac{2}{\sigma}-1\right)} \underbrace{P_{p-2}(Q) \varepsilon_{m}}_{\widetilde{\varepsilon}_{m+p-2}}
\end{aligned}
$$

where: $\widetilde{\varepsilon}_{m+p}=\frac{4}{\sigma} \alpha_{p} Q \widetilde{\varepsilon}_{m+p-1}-2 \alpha_{p} \widetilde{\varepsilon}_{m+p-1}-\beta_{p} \widetilde{\varepsilon}_{m+p-2}$
with: $\left\{\begin{array}{l}\alpha_{p}=\frac{1 \sigma}{22-\sigma} \quad \beta_{p}=0 \quad \text { if } p=1 \\ \alpha_{p}=\frac{c h((p-1) \gamma)}{c h(p \gamma)} \quad \beta_{p}=\frac{\operatorname{ch}((p-2) \gamma)}{c h(p \gamma)} \quad \text { if } p>1\end{array}\right.$ and $\gamma=\operatorname{argch}\left(\frac{2}{\sigma}-1\right)$
Given that: $\widetilde{\varepsilon}_{m+p}=\widetilde{\psi}^{m+p}-\psi$ and $\varepsilon_{m+p}=\psi^{m+p}-\psi$
where:

$$
\widetilde{\psi}^{m+p}=\frac{4}{\sigma} \alpha_{p} Q \widetilde{\psi}^{m+p-1}-2 \alpha_{p} \widetilde{\psi}^{m+p-1}-\beta_{p} \widetilde{\psi}^{m+p-2}-\left(\frac{4}{\sigma} \alpha_{p} Q-2 \alpha_{p} I-\beta_{p} I-I\right) \psi
$$

With the normalization condition of $P_{m}(1)=1$, the last term of the previous equation cancels out. It thus reduces to:

$$
\widetilde{\psi}^{m+p}=\frac{4}{\sigma} \alpha_{p} Q \widetilde{\psi}^{m+p-1}-2 \alpha_{p} \widetilde{\psi}^{m+p-1}-\beta_{p} \widetilde{\psi}^{m+p-2}
$$

The estimation of the dominance ratio $\sigma$ is carried out as follows: after a first cycle of initial power iterations, a first estimate is computed:

$$
\widehat{\sigma}=\frac{\left\|\Psi^{m+p}-\Psi^{m+p-1}\right\|}{\left\|\Psi^{m+p-1}-\Psi^{m+p-2}\right\|}
$$

This estimate is updated at the end of each acceleration cycle. The error is then computed $E=\frac{\left\|\Psi^{m+p}-\Psi^{m+p-1}\right\|}{\left\|\Psi^{m+1}-\Psi^{m}\right\|}$ and the new estimate for the next cycle $\widehat{\sigma}^{\prime}$ is calculated:

$$
\begin{aligned}
& \text { If } E<\frac{1}{\operatorname{ch}((p-1) \gamma)} \text { then } \widehat{\sigma}^{\prime}=\frac{\widehat{\sigma}}{2}\left[\cos \left(\frac{\arccos (E \operatorname{ch}(p \gamma-\gamma))}{p-1}\right)+1\right] \\
& \text { If } E>\frac{1}{\operatorname{ch}((p-1) \gamma)} \text { then } \widehat{\sigma}^{\prime}=\frac{\widehat{\sigma}}{2}\left[\operatorname{ch}\left(\frac{\arg \operatorname{ch}(E \operatorname{ch}(p \gamma-\gamma))}{p-1}\right)+1\right]
\end{aligned}
$$

When the new estimate, $\widehat{\sigma}^{\prime}$, which is normally close to the ratio $\lambda_{0} / \lambda_{1}$, is greater than 1 , the Chebyshev acceleration is temporarily suspended to carry out a cycle of power iterations (approximately 5) and so on.

### 18.4 Finite Difference Method

(Mitchell and Griffith 1980; Planchard 1995, p. 126; Strang and Fix 1973, p. 16)

### 18.4.1 Formalism

The numerical discretization of Eq. (18.1) leads to a leakage term $\left(\operatorname{div}\left(D_{g} \overrightarrow{\operatorname{grad}} \Phi_{g}\right)\right)$ of second order with respect to the space variable. The Finite Difference (FD) method consists in discretizing the continuous problem in a discrete one in which the flux is calculated at specific positions in the reactor. Marchuk and Shaidurov (1983) and Godunov and Ryabenki (1964) thoroughly describe the mathematical aspects of the finite difference method, particularly the order of convergence of the method [see also (Clark and Hansen 1964, p. 75)]. The simplest approach assumes that the neutron quantities are known at the same positions where the flux is to be solved for. For example, (Stacey 2001, p. 82; Clark and Hansen 1964, p. 149; Walter and Reynolds 1981, p. 111) in 1D radial geometry for fast reactors:

Given that $\Delta x_{i} \equiv x_{i+1}-x_{i}$ and $\Delta x_{i-1} \equiv x_{i}-x_{i-1}$ (Fig. 18.5) and the diffusion equation is integrated over a control volume $\left[x_{i-1 / 2}, x_{i+1 / 2}\right]$. This is called Central Finite Differences. ${ }^{3}$

[^367]Fig. 18.5 Finite Differences in 1D

```
In 1D
        ln 1D
```

                                    \(\longrightarrow x\)
    

- Flux discretization points
- Neutron coefficient discretization points

$$
\int_{x_{i-1}-2}^{x_{i-1} / 2}\left[\frac{1}{v_{g}} \frac{\partial \Phi_{g}}{\partial t}-\operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}\right)+\Sigma_{t, g} \Phi_{g}-\chi_{g} \sum_{g^{\prime}=1}^{G} \nu \Sigma_{f, g^{\prime}} \Phi_{g^{\prime}}-\sum_{g^{\prime}=1}^{G} \Sigma_{s, g^{\prime} \rightarrow g} \Phi_{g^{\prime}}\right] d x=0
$$

Each term in the integral is then substituted by its approximation in Finite Difference:

$$
\left\{\begin{array}{c}
\int_{x_{i-1 / 2}}^{x_{i-1 / 2}} \Sigma_{g} \Phi_{g} d x \approx \Sigma_{g}^{i} \Phi_{g}^{i} \Delta x_{i} \forall \Sigma_{g} \\
\left.\int_{x_{i-1 / 2}}^{x_{i-1 / 2}} \operatorname{div}\left(D_{g} \overrightarrow{g r a d} \Phi_{g}\right) d x \approx D_{g} \frac{d \Phi_{g}}{d x}\right|_{i+1 / 2}-\left.D_{g} \frac{d \Phi_{g}}{d x}\right|_{i-1 / 2} \\
\approx \frac{D_{g}^{i+1}+D_{g}^{i} \Phi_{g}^{i+1}-\Phi_{g}^{i}}{2}-\frac{D_{g}^{i}+D_{g}^{i-1} \Phi_{g}^{i}-\Phi_{g}^{i-1}}{2}
\end{array}\right.
$$

Hence, a system of linear equations of unknown $\Phi_{g}^{i}$ is obtained, for which the boundary conditions ( $\Phi_{g}^{1}=0$ and $\Phi_{g}^{n}=0$ for example) or Robin boundary conditions (see equation below) are required.

$$
\Phi_{g}+3 D_{g} \quad \lambda_{g} \frac{d \Phi_{g}}{d n}=0
$$

The Finite Volume method is an alternative approach and consists in calculating the flux at the vertices of a calculation mesh in which the neutron quantities (diffusion coefficient, cross sections) are assumed constant in the mesh. By extension, the neutron quantities are said to be known at the "center of the mesh", which, although a simplification, is nevertheless useful for understanding. Hence, $\Phi(i, j, k)$ denotes the neutron flux at the vertex $(i, j, k)$ whereas $\Sigma(i, j, k)$ denotes the neutron quantity in the mesh $\left[x_{i}, x_{i+1}\right] \times\left[y_{j}, y_{j+1}\right] \times\left[z_{k}, z_{k+1}\right]$ the volume of which is given by $\Delta x_{i} . \Delta y_{j} . \Delta z_{k}$ (Fig. 18.6).

The finite volume method at the "vertex" consists in integrating the equation on an elementary volume surrounding the flux. The elementary volume considered is


Fig. 18.6 Discretization in the finite difference method
centered on the vertex $(i, j, k)$ across the range $\left[x_{i-1 / 2}, x_{i+1 / 2}\right] \times\left[y_{j-1 / 2}, y_{j+1 / 2}\right] \times$ $\left[z_{k-1 / 2}, z_{k+1 / 2}\right]$. The $z$-axis oriented in the same direction as the insertion of the control rods.

In $2 D$, the reaction rates and the source term are given by the contribution of 4 half-cells (without the energy-group indices for the sake of concision):

$$
\begin{aligned}
& \iint_{\text {Control }} \Sigma \Phi d^{2} r=\frac{\Phi(i, j)}{4} \sum_{i^{\prime}=i}^{i^{\prime}=i+1} \sum_{j^{\prime}=j}^{j^{\prime}=j+1} \Sigma\left(i^{\prime}, j^{\prime}\right) \Delta x_{i^{\prime}} \Delta y_{j^{\prime}} \\
& \text { surface }
\end{aligned}
$$

In $3 D$, applying the same principles as in $2 D$, summing is performed for the contributions from two planes of axial meshes, i.e. 8 half-cells:

$$
\begin{aligned}
& \iiint_{\text {Control }} \Sigma \Phi d^{3} r=\frac{\Phi(i, j, k)}{8} \sum_{i^{\prime}=i}^{i^{\prime}=i+1} \sum_{j^{\prime}=j}^{j^{\prime}=j+1} \sum_{k^{\prime}=k}^{k^{\prime}=k+1} \Sigma\left(i^{\prime}, j^{\prime}, k^{\prime}\right) \Delta x_{i^{\prime}} \Delta y_{j^{\prime}} \Delta z_{k^{\prime}} \\
& \text { volume }
\end{aligned}
$$

We can employ the same expressions at the boundaries of the core assuming that the neutron quantities in the required regions are worth zero, which is equivalent to defining the limits of integration for the volume integrals differently. The flux gradient is approximated by a simple finite difference method as seen in the $1 D$ example. The derivative in $x$ for the flux at the center of the meshes is thus expressed as:

$$
\frac{\partial \Phi}{\partial x}(i-1 / 2, j, k)=\frac{\Phi(i, j, k)-\Phi(i-1, j, k)}{\Delta x_{i}}
$$

This is similar to the evaluation of the currents at the center of the meshes:

$$
\begin{aligned}
\iint_{\partial V_{i j}}(D \overrightarrow{\operatorname{grad}} \Phi) \cdot \vec{n} d^{2} r= & \int_{y_{j}}^{y_{j+1}} D\left(\frac{\partial \Phi}{\partial x}(i+1 / 2)-\frac{\partial \Phi}{\partial x}(i-1 / 2)\right) d y \\
& +\int_{x_{i}}^{x_{i+1}} D\left(\frac{\partial \Phi}{\partial y}(j+1 / 2)-\frac{\partial \Phi}{\partial y}(j-1 / 2)\right) d x
\end{aligned}
$$

with:

$$
\left\{\begin{array}{l}
\int_{y_{j}}^{y_{j+1}} D \frac{\partial \Phi}{\partial x}(i+1 / 2) d y=\frac{\Phi(i+1, j)-\Phi(i, j)}{\Delta x_{i+1}}\left[D_{i+1, j} \frac{\Delta y_{j}}{2}+D_{i+1, j+1} \frac{\Delta y_{j+1}}{2}\right] \\
\int_{x_{i}}^{x_{i+1}} D \frac{\partial \Phi}{\partial y}(j+1 / 2) d x=\frac{\Phi(i, j+1)-\Phi(i, j)}{\Delta y_{j+1}}\left[D_{i, j+1} \frac{\Delta x_{i}}{2}+D_{i+1, j+1} \frac{\Delta x_{i+1}}{2}\right]
\end{array}\right.
$$

$\partial V_{i j}$ being the outer surface of the control volume, which is the perimeter of the shaded zone in Fig. 18.7. Thus, in 2D:


Fig. 18.7 Definition of control volume in 2D

$$
\left.\left.\left.\begin{array}{rl}
\iint_{\partial V_{i j}}(D \vec{\nabla} \varphi) \cdot \vec{n} d^{2} r= & -\left(\sum_{i^{\prime}=i}^{i+1} \sum_{j^{\prime}=j}^{j+1} \frac{D_{i^{\prime}, j^{\prime}}}{2}\left(\frac{\Delta y_{j^{\prime}}}{\Delta x_{i^{\prime}}}+\frac{\Delta x_{i^{\prime}}}{\Delta y_{j^{\prime}}}\right)\right) \Phi(i, j) \\
& +\sum_{\substack{i^{\prime}=i-1 \\
i^{\prime} \neq i}}^{i+1}\left[\left(\sum_{i^{\prime}=j}^{j+1} \frac{D_{\max \left(i i^{\prime}\right), j^{\prime}}}{2} \Delta y_{j^{\prime}}\right.\right. \\
\left.\Delta x_{\max \left(i, i^{\prime}\right)}\right)
\end{array}\right) \Phi\left(i^{\prime}, j\right)\right]\right]
$$

And by generalizing to $3 D$, the diffusion term is written as:

$$
\begin{aligned}
\iint_{\partial V_{i j k}}(D \vec{\nabla} \varphi) \cdot \vec{n} d^{2} r & =-\left(\sum_{i^{\prime}=i}^{i+1} \sum_{j^{\prime}=j}^{j+1} \sum_{k^{\prime}=k}^{k+1} \frac{D_{i^{\prime}, j^{\prime}, k^{\prime}}}{4}\left(\frac{\Delta y_{j^{\prime}} \Delta z_{k^{\prime}}}{\Delta x_{i^{\prime}}}+\frac{\Delta x_{i^{\prime}} \Delta z_{k^{\prime}}}{\Delta y_{j^{\prime}}}+\frac{\Delta x_{i^{\prime}} \Delta y_{j^{\prime}}}{\Delta z_{k^{\prime}}}\right)\right) \Phi(i, j, k) \\
& +\sum_{\substack{i^{\prime}=i-1}}^{i+1}\left[\left(\sum_{i^{\prime}==}^{j+1} \sum_{k^{\prime}=k}^{k+1} \frac{D_{\max \left(i, i^{\prime}\right), j^{\prime}, k^{\prime}}}{4} \frac{\Delta y_{j^{\prime}} \Delta z_{k^{\prime}}}{\Delta x_{\max \left(i, i^{\prime}\right)}}\right) \Phi\left(i^{\prime}, j, k\right)\right] \\
& +\sum_{j^{\prime}=j-1}^{j+1}\left[\left(\sum_{i^{\prime}=i=i}^{i+1} \sum_{k^{\prime}=k}^{k+1} \frac{D_{i^{\prime}, \max \left(j, j^{\prime}\right), k^{\prime}}}{4} \frac{\Delta x_{i^{\prime}} \Delta z_{k^{\prime}}}{\Delta y_{\max }\left(j, j^{\prime}\right)}\right) \Phi\left(i, j^{\prime}, k\right)\right] \\
& +\sum_{j^{\prime} \neq j}^{k+1}\left[\left(\sum_{i^{\prime}=i}^{i+1} \sum_{j^{\prime}=i}^{j+1} \frac{D_{i^{\prime}, j^{\prime}, \max \left(k, k^{\prime}\right)}}{4} \frac{\Delta x_{i^{\prime}} \Delta y_{j^{\prime}}}{\Delta z_{\max \left(j, j^{\prime}\right)}}\right) \Phi\left(i, j, k^{\prime}\right)\right]
\end{aligned}
$$

In kinetics, the time derivative is discretized using a Taylor expansion at order 1:

$$
\frac{\partial \Phi}{\partial t}\left(t_{n+1}\right) \approx \frac{\Phi\left(t_{n+1}\right)-\Phi\left(t_{n}\right)}{\Delta t_{n}}
$$

The following volume integrals must thus be evaluated:

$$
\left\{\begin{array}{l}
\iint_{V_{i j}} \frac{1 \Phi}{v \Delta t_{n}} d^{3} r=\frac{\Phi(i, j)}{v(i, j) \Delta t_{n}} \frac{\left(\Delta x_{i}+\Delta x_{i+1}\right)\left(\Delta y_{j}+\Delta y_{j+1}\right)}{4} \quad \text { in } 2 D \\
\iiint_{V_{i j k}} \frac{1 \Phi}{v \Delta t_{n}} d^{3} r=\frac{\Phi(i, j, k)}{v(i, j, k) \Delta t_{n}} \frac{\left(\Delta x_{i}+\Delta x_{i+1}\right)\left(\Delta y_{j}+\Delta y_{j+1}\right)\left(\Delta z_{k}+\Delta z_{k+1}\right)}{8} \quad \text { in } 3 D
\end{array}\right.
$$

### 18.4.2 Boundary Conditions

The above expressions are valid for any position within the active core. For a position $(i, j, k)$ situated at the boundary, Robin boundary conditions are applied:

$$
\Phi+3 D \quad \lambda \frac{d \Phi}{d n}=0
$$

Here, $n$ is the external normal worth $x, y$ or $z$ according to the position considered. For example, integration over the $O x$ axis is carried out only on the range $\left[x_{n-1 / 2}, x_{n}\right]$, since beyond this, the flux is assumed to be zero. This is equivalent to considering that the cross sections in the reaction rates integrals are worth zero for meshes outside the pattern. For the leakage term, the boundary condition is applied to the normal derivative of the flux. For instance, in direction $x$, the following is obtained:

$$
\int_{y_{j}}^{y_{j+1}} D \frac{\partial \Phi}{\partial x}\left(x=x_{n}\right) d y=\int_{y_{j}}^{y_{j+1}}-\frac{\Phi}{3 \lambda}\left(x=x_{n}\right) d y=\Phi(i, j)\left(\frac{\Delta y_{j}}{6 \lambda_{i+1, j}}+\frac{\Delta y_{j+1}}{6 \lambda_{i+1, j+1}}\right)
$$

And likewise for the terms in the other directions. Therefore, in 2D:

$$
\begin{aligned}
\iint_{\partial V_{i j}}(D \overrightarrow{\operatorname{grad}} \Phi) \cdot \vec{n} d^{2} r & =-\left[\sum_{j^{\prime}=j}^{j+1}\left(\frac{D_{i, j^{\prime}}}{2}\left(\frac{\Delta y_{j^{\prime}}}{\Delta x_{i}}+\frac{\Delta x_{i}}{\Delta y_{j^{\prime}}}\right)+\frac{\Delta y_{j^{\prime}}}{6 \lambda_{i+1, j^{\prime}}}\right)\right] \Phi(i, j) \\
& +\left(\sum_{j^{\prime}=j}^{j+1} \frac{D_{i, j^{\prime}} \Delta y_{j^{\prime}}}{2 \Delta x_{i}}\right) \Phi(i-1, j) \\
& +\sum_{\substack{j^{\prime}=j-1 \\
j^{\prime} \neq j}}^{j+1}\left[\left(\frac{D_{i, \max \left(j, j^{\prime}\right)} \Delta x_{i}}{2 y_{\max \left(j, j^{\prime}\right)}}\right) \Phi\left(i, j^{\prime}\right)\right]
\end{aligned}
$$

and in $3 D$ :

$$
\begin{aligned}
& \iint_{\partial V_{i j k}}\left(D \overrightarrow{\operatorname{grad} \Phi) \cdot \vec{n} d^{2} r=}\right. \\
& \quad-\left(\sum_{i^{\prime}=j}^{j+1} \sum_{k^{\prime}=k}^{k+1}\left[\frac{D_{i, j^{\prime}, k^{\prime}}}{4}\left(\frac{\Delta y_{j^{\prime}} \Delta z_{k^{\prime}}}{\Delta x_{i}}+\frac{\Delta x_{i} \Delta z_{k^{\prime}}}{\Delta y_{j^{\prime}}}+\frac{\Delta x_{i} \Delta y_{j^{\prime}}}{\Delta z_{k^{\prime}}}\right)+\frac{\Delta y_{j^{\prime}} \Delta z_{k^{\prime}}}{12 \lambda_{i+1, j^{\prime}, k^{\prime}}}\right]\right) \Phi(i, j) \\
& \quad+\left(\sum_{j^{\prime}=j}^{j+1} \sum_{k^{\prime}=k}^{k+1} \frac{D_{i, j^{\prime}, k^{\prime}}}{4} \frac{\Delta y_{j^{\prime}} \Delta z_{k^{\prime}}}{\Delta x_{i}}\right) \Phi(i-1, j, k) \\
& \quad+\sum_{j^{\prime}=j-1}^{j+1}\left[\left(\sum_{k^{\prime}=k}^{k+1} \frac{D_{i, \max \left(j, j^{\prime}\right), k^{\prime}}}{4} \frac{\Delta x_{i} \Delta z_{k^{\prime}}}{\Delta y_{\max \left(j, j^{\prime}\right)}}\right) \Phi\left(i, j^{\prime}, k\right)\right] \\
& \quad+\sum_{k^{\prime}=k-1}^{k+1}\left[\left(\sum_{j^{\prime}=i}^{j+1} \frac{D_{i, j^{\prime}, \max \left(k, k^{\prime}\right)}}{4} \frac{\Delta x_{i} \Delta y_{j^{\prime}}}{\Delta z_{\max \left(j, j^{\prime}\right)}}\right) \Phi\left(i, j, k,,^{\prime}\right)\right]
\end{aligned}
$$

The term in time is discretized as:

$$
\begin{cases}\iint_{V_{i j}} \frac{1}{v} \frac{\Phi}{\Delta t_{n}} d^{2} r=\frac{\Phi(i, j)}{v(i, j) \Delta t_{n}} \frac{\Delta x_{i}\left(\Delta y_{j}+\Delta y_{j+1}\right)}{4} & \text { in } 2 D \\ \iiint_{V_{i j k}} \frac{1}{v} \frac{\Phi}{\Delta t_{n}} d^{3} r=\frac{\Phi(i, j, k)}{v(i, j, k) \Delta t_{n}} \frac{\Delta x_{i}\left(\Delta y_{j}+\Delta y_{j+1}\right)\left(\Delta z_{k}+\Delta z_{k+1}\right)}{8} & \text { in } 3 D\end{cases}
$$

Similar expressions are obtained for the boundaries in $y$ and $z$, as well as the 'edges' and the 'corners' of the domain (double and triple boundary conditions respectively).

### 18.4.3 Matrix Form

After integration over the control volumes, the equations can be written in their matrix form as shown earlier for the stationary equation (Clark and Hansen 1964, p. 170). The two-group matrices $A_{1}$ and $A_{2}$ should then be inverted ( $A_{1}$ and $A_{2}$ in kinetics with $A_{g}^{\prime}=\left(v_{g} \Delta t_{g}\right)^{-1} I-A_{g}$ for $g=1$ or 2). This can be done using an $L U$ factorization and a Jacobi method, combined with a Block Gauss-Seidel method (Planchard 1995, p. 253; Varga 1962). Similarly, acceleration of the convergence using a conjugate gradient method (Gastinel 1966, p. 181; Jacoby et al. 1972, p. 97)

Fig. 18.8 Shape of the matrix: example with 3 planes and 4 nodes in $x$ and $y$

may be carried out in both stationary and kinetic cases. The terms on the RHS stem either from the previous time iteration or from the previous outer iteration (coupling iteration). In the kinetic case, these iterations are used to compute the precursor concentrations, $C_{i}$, as a function of the fluxes just calculated. Spatial discretization at each node of the mesh involves the six adjacent nodes (Fig. 18.8).

The square matrices of operators $A_{1}$ and $A_{2}$ are positive-definite and contain 7 non-zero diagonals. In $2 D$ and $l D$, these matrices have 5 and 3 non-zero diagonals respectively. In the general $3 D$ case, the non-zero diagonals are the principal $P D$, the two adjacent diagonals (above and below $D P$ ) $D X^{-}$and $D X^{+}$for the spatial discretization in the $O x$ axis, the two diagonals $D Y^{-}$and $D Y^{+}$located at the $+n_{x}$ and $-n_{x}$ cells (where $n_{x}$ is the number of nodes in $x$ ) the discretization in the $O y$ axis, and the two diagonals $D Z^{-}$and $D Z^{+}$located at $+n_{x} . n_{y}$ and $-n_{x} . n_{y}$ cells (where $n_{y}$ is the number of nodes in $y$ ) for the terms in the $O z$ axis.

### 18.5 Nodal Methods

(Planchard 1995, p. 141; Stacey 1967; Stacey 2001, p. 545)
A large number of numerical methods may be classified as Nodal Methods (NM also known as Nodal Expansion Methods $=N E M$ ). The general principles of these methods, which originated in the 1970s (from the works of Finneman, Henry,

Kord Smith, ${ }^{4}$ Koebke, etc.), consist in discretizing the reactor core in meshes of relatively large size (nodes) with uniform medium where the fluxes are considered as average values. The flux is assumed to have an intra-nodal form (polynomial or some other function) and the coefficients are calculated whilst ensuring that the flux and current verify the continuity equations. The method is called a summation method if the flux is obtained by summing functions in the vector space. This technique allows a high precision on the reconstruction of the intra-nodal fluxes, ${ }^{5,6}$ without being costly as the Finite Difference method, which requires refined mesh for equivalent precision. Other methods known as analytical methods also exist, and rather than the flux, it is the RHS of the diffusion equation that is integrated along a direction (this is called "transverse diffusion equation"). ${ }^{7}$ These methods are highly ingenious since once the coefficients are known, the flux can be calculated at any point in the mesh. This is particularly useful for determining the hot spot for instance. Further, nodal methods have the same precision as finite difference methods with coarser meshes. For example, one radial cell per assembly is sufficient in nodal methods whereas 16 would be required for the finite difference method, thereby explaining its relative spread in the 1990s due to the gain in calculation times. Mathematical studies have shown the nodal methods to be very close to finite element methods.

[^368]

[^369]
### 18.5.1 Nodal Method of Order 4

We will now illustrate the principles of the nodal methods with the order 4 of the method as implemented in the EDF calculation scheme. ${ }^{8}$ Most nodal methods hinge more or less on the same ideas. Let us examine a reactor meshed with cells indexed by $K$ in which neutron quantities are assumed constant. For practical purposes, the center of the cell $K$ is taken as the origin of the local frame of reference and hence defines the cell with its dimensions:

$$
K=\left[-\frac{h_{x}}{2},+\frac{h_{x}}{2}\right] \times\left[-\frac{h_{y}}{2},+\frac{h_{y}}{2}\right] \times\left[-\frac{h_{z}}{2},+\frac{h_{z}}{2}\right]
$$

The flux is defined in the cell for group $g$ as $\Phi_{g}(x, y, z)$, along with the following (Fig. 18.9):

[^370]
(Courtesy Noceir)


Fig. 18.9 Representation of discretization in $2 D$ and $3 D$ : definition of notations

In $2 D$, the neutron balance equation per cell is obtained by integrating the diffusion equation over cell $K$ :

$$
\frac{1}{h_{x}}\left\{J_{x+}-J_{x-}\right\}+\frac{1}{h_{y}}\left\{J_{y+}-J_{y-}\right\}+\frac{1}{h_{z}}\left\{J_{z+}-J_{z-}\right\}+\Sigma \bar{\Phi}=\bar{S}
$$

with: $\bar{S}=\frac{1}{h_{x} h_{y} h_{z}} \int_{K} S(x, y, z) d x d y d z$
This equation relates the average flux to the average currents at the interfaces. It is a fundamental equation that must be verified whichever type of nodal method used. It is also possible to integrate along the two directions (one in 2D). For instance, integrating along $y$ and $z$ leads to the following equation:

$$
\begin{equation*}
\text { Transverse equation : } \frac{d}{d x} J_{x}(x)+\Sigma \Phi_{x}(x)=S_{x}(x)-F_{x}(x) \tag{18.3}
\end{equation*}
$$

where $F_{x}(x)$ and $S_{x}(x)$ are the leakage and source terms, respectively, in the $x$ direction:

Substituting the transverse current by its expression, this equation can also be written as a second-order differential equation:

$$
\frac{d}{d x}\left(D \frac{d \Phi_{x}(x)}{d x}\right)+\Sigma \Phi_{x}(x)=S_{x}(x)-F_{x}(x)
$$

The transverse leakage values are given in terms of their average value and the average currents on the interfaces of cell $K$ :

$$
\frac{1}{h_{x}} \int_{-\frac{h_{x}}{2}}^{+\frac{h_{x}}{2}} F_{x}(x) d x=\bar{F}_{x}=\frac{1}{h_{y}}\left(J_{y+}-J_{y-}\right)+\frac{1}{h_{z}}\left(J_{z+}-J_{z-}\right)
$$

The development of nodal methods based on the solution of the transverse equations in each direction is due to the simple fact that it is easier to solve an equation in one dimension rather than one in two or three dimensions. This approach is called the Transverse-Integrated Nodal Method (TINM) (Stacey 2001, p. 547). Nevertheless, it requires knowing the transverse leakages. The information is obtained on mono-dimensional fluxes only and does not allow rigorous calculation of the multi-dimensional value at any point in the domain. In the case of an order- 4 method, the flux is approximated by a polynomial without crossed terms, with degree 4 in $x$ and $y$, and degree 2 in $z$ :

$$
\begin{aligned}
\Phi(x, y, z)=a_{0} & +a_{1} f_{1}(x)+a_{2} f_{2}(x)+a_{3} f_{3}(x)+a_{4} f_{4}(x) \\
& +b_{1} f_{1}(y)+b_{2} f_{2}(y)+b_{3} f_{3}(y)+b_{4} f_{4}(y) \\
& +c_{1} f_{1}(z)+c_{2} f_{2}(z)
\end{aligned}
$$

where: $\left\{\begin{array}{l}f_{1}(\xi)=\frac{x}{h_{x}}=\xi \quad f_{3}(\xi)=\xi\left(\xi^{2}-\frac{1}{4}\right) \\ f_{2}(\xi)=3 \xi^{2}-\frac{1}{4} \quad f_{4}(\xi)=\left(\xi^{2}-\frac{1}{4}\right) \quad\left(\xi^{2}-\frac{1}{20}\right)\end{array}\right.$

Several studies have shown that degree 2 is sufficient given that the flux is less perturbed in the axial direction than the radial one in PWR (except at the grids which, however, have an influence on a small height, or due to the presence of rods whose permanent insertion in the core is not recommended). The basis functions $f_{i}$ are introduced to simplify the computations required for discretization. They are chosen such that:

$$
\int_{-\frac{h i}{2}}^{-\frac{h x}{2}} f_{i}(\xi) d \xi=0 \quad \forall i \text { and } f_{i}\left( \pm \frac{1}{2}\right)=0 \quad \text { for } i=3 \text { or } 4
$$

Which, by transverse integration, give:

$$
\Phi_{x}(x)=a_{0}+a_{1} f_{1}(x)+a_{2} f_{2}(x)+a_{3} f_{3}(x)+a_{4} f_{4}(x) \text { with }\left\{\begin{array}{l}
a_{0}=\bar{\Phi} \\
a_{1}=\Phi_{x+}-\Phi_{x-} \\
a_{2}=\Phi_{x+}+\Phi_{x-}-2 \bar{\Phi}
\end{array}\right.
$$

Coefficients $a_{3}$ and $a_{4}$ are determined by weighting the diffusion equation by weight functions $Q_{1}$ and $Q_{2}$, which are function of $x$ only:

$$
\left\langle Q_{i},-\operatorname{div}(\overrightarrow{\operatorname{grad}} \Phi)\right\rangle+\Sigma\left\langle Q_{i}, \Phi\right\rangle=\left\langle Q_{i}, S\right\rangle
$$

where: $\left\langle Q_{i}, \Phi\right\rangle=\frac{1}{h_{x} h_{y} h_{z}} \int_{K} Q_{i} \Phi d x d y d z$ for $i=1,2$
If $Q_{1}=f_{1}$ and $Q_{2}=f_{2}$, for $i=1,2$, the following is obtained:

$$
\begin{aligned}
\left\langle f_{i},-\operatorname{div}(\overline{\operatorname{grad}} \Phi)\right\rangle & =\frac{1}{h_{x} h_{y}} \int_{K}-\operatorname{div}(\overline{\operatorname{grad}} \Phi) f_{i}(x) d x d y \\
& =-\frac{D}{h_{x} h_{y}}\left\{\int_{K}\left(\frac{\partial^{2} \Phi}{\partial x^{2}}+\frac{\partial^{2} \Phi}{\partial y^{2}}+\frac{\partial^{2} \Phi}{\partial z^{2}}\right) f_{i}(x) d x d y\right\}
\end{aligned}
$$

As $\Phi$ is polynomial with no crossed terms, then $\frac{\partial^{2} \Phi}{\partial y^{2}}$ and $\frac{\partial^{2} \Phi}{\partial z^{2}}$ are independent of $x$ and, thus:

The only non-zero integral is computed as:

$$
\left\{\begin{array}{l}
\left\langle f_{1},-\operatorname{div}(\operatorname{D} \overrightarrow{\operatorname{grad}} \Phi)\right\rangle=-\frac{D}{h_{x} h_{y}}\left\{\int_{K}\left(\frac{\partial^{2} \Phi}{\partial x^{2}}\right) f_{1}(x) d x d y\right\}=\frac{1}{2 h_{x}}\left(J_{x+}+J_{x-}\right)+\frac{D}{h_{x}^{2}}\left(\Phi_{x+}-\Phi_{x-}\right) \\
\left\langle f_{2},-\operatorname{div}(\overrightarrow{\operatorname{Drad}} \Phi)\right\rangle=-\frac{D}{h_{x} h_{y}}\left\{\int_{K}\left(\frac{\partial^{2} \Phi}{\partial x^{2}}\right) f_{2}(x) d x d y\right\}=\frac{1}{2 h_{x}}\left(J_{x+}-J_{x-}\right)+\frac{3 D}{h_{x}^{2}}\left(\Phi_{x+}+\Phi_{x-}-2 \bar{\Phi}\right)
\end{array}\right.
$$

Therefore, the weighted balance equations are:

$$
\left\{\begin{array}{l}
\frac{1}{2 h_{x}}\left(J_{x+}+J_{x-}\right)+\frac{D}{h_{x}^{2}}\left(\Phi_{x+}-\Phi_{x-}\right)+\Sigma \underbrace{\left\langle f_{1}, \Phi\right\rangle}_{\bar{\Phi}_{x 1}}=\underbrace{\overline{\left\langle f_{1}, S\right\rangle}}_{\bar{S}_{x 1}} \\
\frac{1}{2 h_{x}}\left(J_{x+}-J_{x-}\right)+\frac{3 D}{h_{x}^{2}}\left(\Phi_{x+}+\Phi_{x-}-2 \bar{\Phi}\right)+\Sigma \underbrace{\left\langle f_{2}, \Phi\right\rangle}_{\bar{\Phi}_{x 2}}=\underbrace{\overline{\left\langle f_{2}, S\right\rangle}}_{\bar{S}_{x 2}}
\end{array}\right.
$$

$\bar{\Phi}_{x 1}$ and $\bar{\Phi}_{x 2}$ are calculated by expanding the flux $\Phi$ in its polynomial form:

$$
\left\langle f_{i}(x), \Phi\right\rangle=\sum_{j=1}^{4} \frac{a_{j}}{h_{x} h_{y}} \int_{K} f_{i}(x) f_{j}(x) d x d y
$$

This expression is written with scalar products of the base functions:

$$
\begin{aligned}
& \int_{-\frac{h_{x}}{2}}^{++\frac{h_{x}}{2}} f_{1}(x) f_{1}(x) d x=\frac{h_{x}}{12}, \int_{-\frac{h_{x}}{2}}^{+\frac{h_{x}}{2}} f_{1}(x) f_{3}(x) d x=-\frac{h_{x}}{120}, \int_{-\frac{h_{x}}{2}}^{++\frac{h_{x}}{2}} f_{1}(x) f_{j}(x) d x=0 \text { for } j=2 \text { or } 4 \\
& \int_{-\frac{h_{x}}{2}}^{+\frac{h_{x}}{2}} f_{2}(x) f_{2}(x) d x=\frac{h_{x}}{20}, \int_{-\frac{h_{x}}{2}}^{+\frac{h_{x}}{2}} f_{2}(x) f_{3}(x) d x=0, \int_{-\frac{h_{x}}{2}}^{+\frac{h_{x}}{2}} f_{2}(x) f_{4}(x) d x=-\frac{h x}{700}
\end{aligned}
$$

The following equations are obtained for the weighted flux:

$$
\left\{\begin{array}{l}
\bar{\Phi}_{x 1}=\frac{1}{12} a_{1}-\frac{1}{120} a_{3} \\
\bar{\Phi}_{x 2}=\frac{1}{20} a_{2}-\frac{1}{700} a_{4}
\end{array}\right.
$$

Also by integration, the transverse currents are:

$$
\left\{\begin{array}{l}
J_{x+}=-\frac{D}{h_{x}}\left\{a_{1}+3 a_{2}+\frac{1}{2} a_{3}+\frac{1}{5} a_{4}\right\} \\
J_{x-}=-\frac{D}{h_{x}}\left\{a_{1}-3 a_{2}+\frac{1}{2} a_{3}-\frac{1}{5} a_{4}\right\}
\end{array}\right.
$$

By substituting the coefficients $a_{i}$ by their expressions in terms of average flux at the interface and the weighted flux, the following coupling of the currents and the flux are obtained:

$$
\left\{\begin{array}{l}
J_{x+}=-\frac{D}{h x}\left\{16 \Phi_{x+}+4 \Phi_{x-}-60 \bar{\Phi}_{x 1}-140 \bar{\Phi}_{x 2}-20 \bar{\Phi}\right\} \\
J_{x-}=-\frac{D}{h x}\left\{-4 \Phi_{x+}-16 \Phi_{x-}-60 \bar{\Phi}_{x 1}+140 \bar{\Phi}_{x 2}+20 \bar{\Phi}\right\}
\end{array}\right.
$$

which is similar to:

$$
\left\{\begin{array}{l}
\Phi_{x+}=-\frac{h_{x}}{60 D}\left\{4 J_{x+}+J_{x-}\right\}+\bar{\Phi}+5 \bar{\Phi}_{x 1}+7 \bar{\Phi}_{x 2} \\
\Phi_{x-}=+\frac{h_{x}}{60 D}\left\{J_{x+}+4 J_{x-}\right\}+\bar{\Phi}-5 \bar{\Phi}_{x 1}+7 \bar{\Phi}_{x 2}
\end{array}\right.
$$

Finally, the equations (in $2 D$ ) with the interface currents as unknowns are obtained:

Neutron balance equation:

$$
\begin{equation*}
\frac{1}{h_{x}}\left\{J_{x+}-J_{x-}\right\}+\frac{1}{h_{y}}\left\{J_{y+}-J_{y-}\right\}+\frac{1}{h_{z}}\left\{J_{z+}-J_{z-}\right\}+\Sigma \bar{\Phi}=\bar{S} \tag{18.4}
\end{equation*}
$$

Weighted balance equations: $\left\{\begin{array}{l}\frac{5}{12 h_{x}}\left(J_{x+}+J_{x-}\right)+\left(\frac{10 D}{h_{x}^{2}}+\Sigma\right) \bar{\Phi}_{x 1}=\bar{S}_{x 1} \\ \frac{7}{20 h_{x}}\left(J_{x+}-J_{x-}\right)+\left(\frac{42 D}{h_{x}^{2}}+\Sigma\right) \bar{\Phi}_{x 2}=\bar{S}_{x 2}\end{array}\right.$

The coupling between cells is ensured via the flux continuity and the average currents at the interface of cell $K$ and its immediate neighbor $K^{\prime}$ :

$$
\left\{\begin{array}{l}
\Phi_{x+}(K)=\Phi_{x-}\left(K^{\prime}\right) \\
J_{x+}(K)=J_{x-}\left(K^{\prime}\right)
\end{array}\right.
$$

It should, however, be noted that continuity is not guaranteed at all points at the interface (only the average flux and currents are retained). At the boundaries, Robin boundary conditions are applied. For the left boundary of the reactor, the following is written:

$$
J_{x-}=+\frac{h_{x}}{60 D}\left\{J_{x+}+4 J_{x-}\right\}+\bar{\Phi}-5 \bar{\Phi}_{x 1}+7 \bar{\Phi}_{x 2}=-\frac{\bar{\Phi}_{x-}}{3 \lambda_{-}}
$$

And similarly for the right boundary:

$$
J_{x-}=-\frac{D}{h_{x}}\left\{-4 \Phi_{x+}-16 \Phi_{x-}-60 \bar{\Phi}_{x 1}+140 \bar{\Phi}_{x 2}+20 \bar{\Phi}\right\}=+\frac{\Phi_{x+}}{3 \lambda_{+}}
$$

where $\lambda_{-}$and $\lambda_{+}$are the extrapolation lengths with regard to the left and right edges respectively. When the previous equations are obtained for all the cells K in the mesh, the different interfaces and the boundaries of the domain in all directions, they form a linear system with as many equations as unknowns. This system is written as $A X=B$ where $X$ consists of the vectors $\bar{\Phi}, J_{x+}, \bar{\Phi}_{x 1}$ and $\bar{\Phi}_{x 2}$ along each direction. The $J_{x-}$ terms are replaced with those of the neighboring meshes by continuity considerations (Fig. 18.10).

Matrix $A$ is composed of elementary matrices of the following form:

$$
\left(\begin{array}{cccc}
0 & 0 & 0 & \frac{1}{h_{x}} \\
0 & \left(\frac{10 D}{h_{x}^{2}}+\Sigma\right) & 0 & \frac{5}{12 h_{x}} \\
0 & 0 & \left(\frac{42 D}{h_{x}^{2}}+\Sigma\right) & \frac{7}{20 h_{x}} \\
-1 & -5 & -7 & \left(\frac{h_{x}}{15 D}+\frac{h_{x^{\prime}}}{15 D^{\prime}}\right)
\end{array}\right)
$$

In this expression, the properties of an adjacent cell are written using the prime index ('). The matrix obtained can be made symmetric but is not positive-definite, which can be quite troublesome when seeking to ensure that the flux obtained is

Fig. 18.10 Nodal element of degree 4 with interface currents

positive. An elimination method yields a system that is positive-definite. If $J$ represents the current vector (consisting of average interface currents along all the directions), and $\Phi$ represents the flux vector comprising average and weighted fluxes, for an interface current method, the final system can be written as:

$$
\left(\begin{array}{ll}
M_{1} & M_{2} \\
M_{2}^{t} & M_{3}
\end{array}\right)\binom{J}{\Phi}=\binom{0}{B}
$$

If the flux is eliminated, the following sub-system is obtained:

$$
\left\{\begin{array}{l}
\tilde{A} J=\tilde{B} \\
\tilde{A}=M_{1}-M_{2} M_{3}^{-1} M_{2}^{t} \quad \tilde{B}=-M_{2} M_{3}^{-1} B
\end{array}\right.
$$

The matrix of sub-system $\tilde{A}$ is positive-definite. Indeed, since $M_{1}$ derives from the interface equations, it is a symmetric tri-diagonal matrix with a strictly positive diagonal. Hence, it is positive-definite. $M_{3}$ is written from the balance equations and is thus a diagonal matrix with negative terms only. Therefore, matrix $-M_{2} M_{3}^{-1} M_{2}^{t}$ is symmetric and positive-definite. The sum of two symmetric positive-definite matrices is also symmetric and positive-definite, as for $\tilde{A}$. The average flux values are given by:

$$
\begin{gathered}
\bar{\Phi}=\frac{\bar{S}}{\Sigma}-\frac{1}{\Sigma h_{x}}\left\{J_{x+}-J_{x-}\right\}-\frac{1}{\Sigma h_{y}}\left\{J_{y+}-J_{y-}\right\}-\frac{1}{\Sigma h_{z}}\left\{J_{z+}-J_{z-}\right\} \\
\left\{\begin{array} { l } 
{ \overline { \Phi } _ { x 1 } = \frac { \overline { S } _ { x 1 } } { \sum _ { x 1 } } - \frac { 5 } { 1 2 \Sigma _ { x 1 } h _ { x } } ( J _ { x + } + J _ { x - } ) } \\
{ \overline { \Phi } _ { x 2 } = \frac { \overline { S } _ { x 2 } } { \Sigma _ { x 2 } } - \frac { 7 } { 2 0 \Sigma _ { x 2 } h _ { x } } ( J _ { x + } - J _ { x - } ) }
\end{array} \text { where } \left\{\begin{array}{l}
\Sigma_{x 1}=\Sigma+\frac{10 D}{h_{x}^{2}} \\
\Sigma_{x 2}=\Sigma+\frac{42 D}{h_{x}^{2}}
\end{array}\right.\right.
\end{gathered}
$$

By inserting the expressions in the interface equations, after computation, the following is obtained:

$$
\left\{\begin{array}{l}
\left(\frac{h_{x}}{60 D}-\frac{1}{\sum h_{x}}+\frac{25}{12 \Sigma_{x 1} h_{x}}-\frac{49}{20 \Sigma_{x 2} h_{x}}\right) J_{x-} \\
+\left(\frac{h_{x}}{15 D}+\frac{1}{\Sigma h_{x}}+\frac{25}{12 \Sigma_{x 1} h_{x}}+\frac{49}{20 \Sigma_{x 2} h_{x}}+\frac{h_{x}^{\prime}}{15 D^{\prime}}+\frac{1}{\Sigma^{\prime} h_{x}^{\prime}}+\frac{25}{12 \Sigma_{x 1}^{\prime} h_{x}^{\prime}}+\frac{49}{20 \Sigma_{x 2}^{\prime} h_{x}^{\prime}}\right) J_{x+} \\
+\left(\frac{h x^{\prime}}{60 D^{\prime}}-\frac{1}{\Sigma^{\prime} h_{x}^{\prime}}+\frac{25}{12 \Sigma_{x 1}^{\prime} h_{x}^{\prime}}-\frac{49}{20 \Sigma_{x 2}^{\prime} h_{x}^{\prime}}\right) J_{x+}^{\prime} \\
\quad=\frac{\bar{S}}{\Sigma}-\frac{\bar{S}^{\prime}}{\Sigma^{\prime}}+\frac{5 \bar{S}_{x 1}}{\Sigma_{x 1}}+\frac{5 \bar{S}_{x 1}^{\prime}}{\Sigma_{x 1}^{\prime}}+\frac{7 \bar{S}_{x 2}}{\Sigma_{x 2}}-\frac{7 \bar{S}_{x 2}^{\prime}}{\Sigma_{x 2}^{\prime}} \\
\quad-\frac{1}{\sum h_{y}}\left(J_{y+}-J_{y-}\right)+\frac{1}{\Sigma^{\prime} h_{y}^{\prime}}\left(J_{y+}^{\prime}-J_{y-}^{\prime}\right)-\frac{1}{\sum h_{z}}\left(J_{z+}-J_{z-}\right)+\frac{1}{\Sigma^{\prime} h_{z}^{\prime}}\left(J_{z+}^{\prime}-J_{z-}^{\prime}\right)
\end{array}\right.
$$

Naturally, these calculations must also be carried out for the other components ( $y$ and $z$ ). The resulting equations for $y$ are similar to those obtained for $x$. For $z$ on
the other hand, some simplifications are possible (the $z$ component being of degree 2 instead of 4). Finally, the following equation is obtained:

$$
\begin{aligned}
& \left(\frac{h_{z}}{6 D}-\frac{1}{\Sigma h_{z}}\right) J_{z-}+\left(\frac{h_{z}}{3 D}+\frac{h_{z}^{\prime}}{3 D^{\prime}}+\frac{1}{\Sigma h_{z}}+\frac{1}{\Sigma^{\prime} h_{z}^{\prime}}\right) J_{z+}+\left(\frac{h_{z}^{\prime}}{6 D^{\prime}}-\frac{1}{\Sigma^{\prime} h_{z}^{\prime}}\right) J_{z+}^{\prime} \\
& \quad=\frac{\bar{S}}{\Sigma}-\frac{\bar{S}^{\prime}}{\Sigma^{\prime}}-\frac{1}{\Sigma h_{x}}\left(J_{x+}-J_{x-}\right)+\frac{1}{\Sigma^{\prime} h_{x}^{\prime}}\left(J_{x+}^{\prime}-J_{x-}^{\prime}\right)-\frac{1}{\Sigma h_{y}}\left(J_{y+}-J_{y-}\right)+\frac{1}{\Sigma^{\prime} h_{y}^{\prime}}\left(J_{y+}^{\prime}-J_{y-}^{\prime}\right)
\end{aligned}
$$

These equations, written for all $K$ cells, the different interfaces, on the boundaries of the domain and along all the directions, form two linear systems with as many unknowns as there are equations. The first sub-system has the fluxes as unknowns. The elimination method for fluxes leads to a positive-definite system with half the number of unknowns, and a considerable gain in execution time. It enables legitimate use of convergence theorems on iterative methods concerning positive-definite matrices (Gauss-Seidel, etc.).

### 18.5.2 Quadratic Approximation of Transverse Leakage

The works of Slimane Noceir have shown the limits of convergence of the nodal method of order 4. Increasing the degree of the polynomials in the basis does not increase the order of convergence, which remains in $O\left(h^{2}\right)$. Moreover, with such numerical schemes, transverse leakage (accounting for neutrons leaving the cell in a transverse direction to that considered) across the face of the cells is approximated by constants for each face of a given cell. In more recent schemes, this problem has been solved by keeping the same unknowns, as previously seen, for each face, and by improving the representation of transverse leakage with a quadratic approximation that links neighboring cells. This is now a standard method which improves the approximation. In this approach, the balance equation (Eq. 18.4) is not modified. Evaluation of the coefficients $a_{0}, a_{1}, a_{2}, b_{1}$ and $b_{2}$ of the polynomial expansion of the flux is carried out in the same manner. However, to determine coefficients $a_{3}$, $a_{4}, b_{3}$ and $b_{4}$, the transverse equation (Eq. 18.3) is now weighted rather than the balance equation:

$$
\left\langle-D \frac{d^{2} \Phi_{x}}{d x^{2}}(x), f_{i}(x)\right\rangle+\left\langle\Sigma \Phi_{x}(x), f_{i}(x)\right\rangle=\left\langle S_{x}(x), f_{i}(x)\right\rangle-\left\langle F_{x}(x), f_{i}(x)\right\rangle
$$

After calculation, the following scalar products are obtained:

$$
\left\{\begin{array}{l}
\left\langle-D \frac{d^{2} \Phi_{x}}{d x^{2}}, f_{1}\right\rangle=\frac{1}{2 h_{x}}\left(J_{x+}+J_{x-}\right)+\frac{D}{h_{x}^{2}}\left(\Phi_{x+}-\Phi_{x-}\right) \\
\left\langle-D \frac{d^{2} \Phi_{x}}{d x^{2}}, f_{2}\right\rangle=\frac{1}{2 h_{x}}\left(J_{x+}-J_{x-}\right)+\frac{3 D}{h_{x}^{2}}\left(\Phi_{x+}+\Phi_{x-}-2 \bar{\Phi}\right)
\end{array}\right.
$$

The weighted transverse equations are obtained:

$$
\left\{\begin{array}{c}
\frac{1}{2 h_{x}}\left(J_{x+}+J_{x-}\right)+\frac{D}{h_{x}^{2}}\left(\Phi_{x+}-\Phi_{x-}\right)+\Sigma \bar{\Phi}_{x 1}=\bar{S}_{x 1}-\bar{F}_{x 1} \\
\frac{1}{2 h_{x}}\left(J_{x+}-J_{x-}\right)+\frac{3 D}{h_{x}^{2}}\left(\Phi_{x+}+\Phi_{x-}-2 \bar{\Phi}\right)+\Sigma \bar{\Phi}_{x 2}=\bar{S}_{x 2}-\bar{F}_{x 2}
\end{array}\right.
$$

Therefore, the values of $a_{3}$ and $a_{4}$ (hence, $b_{3}$ and $b_{4}$ ) are given by:

$$
\left\{\begin{array}{l}
\bar{\Phi}_{x 1}=\frac{a_{1}}{12}-\frac{a_{3}}{120} \\
\bar{\Phi}_{x 2}=\frac{a_{2}}{20}-\frac{a_{4}}{700}
\end{array}\right.
$$

The interface currents and flux, which were obtained for the nodal method without quadratic leakage, are still valid. Finally, the discretized equations form the following system:

$$
\left\{\begin{array}{l}
\frac{1}{h_{x}}\left(J_{x+}-J_{x-}\right)+\frac{1}{h_{y}}\left(J_{y+}-J_{y-}\right)+\Sigma \bar{\Phi}=\bar{S} \\
\frac{5}{12 h_{x}}\left(J_{x+}+J_{x-}\right)+\left(\frac{10 D}{h_{x}^{2}}+\Sigma\right) \bar{\Phi}_{x 1}=\bar{S}_{x 1}-\bar{F}_{x 1} \\
\frac{7}{20 h_{x}}\left(J_{x+}-J_{x-}\right)+\left(\frac{42 D}{h_{x}^{2}}+\Sigma\right) \bar{\Phi}_{x 2}=\bar{S}_{x 2}-\bar{F}_{x 2}
\end{array}\right.
$$

To these equations are added the continuity equations, which are unchanged with respect to the nodal methods without quadratic leakage. The differences concern only the weighted balance equations with more terms requiring evaluation. The supplementary coefficients can be expressed as a function of the unknowns of the problem. They do not act as new degrees of freedom. The quadratic approximation of the leakage consists in expanding these quantities on a second-degree polynomial, where the coefficients are expressed in terms of the unknowns of the problem. There are several ways to determine the coefficients of this polynomial: on one hand, by conservation of the average transverse leakage by integration on the current cell for the three adjacent cells, or, on the other hand, by relating the leakage terms to their first-order derivatives at the interface. This method requires solving a tri-diagonal system and is more costly than the former. The average leakage on the three neighboring cells is conserved to avoid worsening the efficiency of the calculation. The polynomial expansion of the flux is written as (the $x$ direction is taken for example):

Formula for the quadratic leakages: $F_{x}(x)=\bar{F}_{x}+F_{1} f_{1}(x)+F_{2} f_{2}(x)$
Where:

$$
\bar{F}_{x}=\frac{1}{h_{x}} \int_{-\frac{h_{x}}{2}}^{\frac{h_{x}}{2}} F_{x}(x) d x
$$

corresponds to the average leakage, $F_{1}$ and $F_{2}$ are the coefficients to be determined and $f_{i}$ are the functions of polynomial basis from the nodal method described previously for the flux.
$F_{1}$ and $F_{2}$ are computed while ensuring that the average leakage of the cells $i-1, i$ and $i+1$ are conserved (Fig. 18.11):

$$
\left\{\begin{array}{l}
\frac{1}{h_{x}^{-}} \int_{h_{x}^{-}} F_{x}(x) d x=\bar{F}_{x}^{-} \\
\frac{1}{h_{x}^{+}} \int_{h_{x}^{+}} F_{x}(x) d x=\bar{F}_{x}^{+}
\end{array}\right.
$$

where: $\bar{F}_{x}^{ \pm}=\bar{F}_{x}+\alpha_{1}^{ \pm} F_{1}+\alpha_{2}^{ \pm} F_{2}$ with: $\alpha_{i}^{ \pm}=\frac{1}{h_{x}^{ \pm}} \int_{h_{x}^{ \pm}} f_{i}(x) d x$
The system to be solved is the following:

$$
\left\{\begin{array}{l}
\alpha_{1}^{+} F_{1}+\alpha_{2}^{+} F_{2}=\bar{F}_{x}^{+}-\bar{F}_{x}=\beta^{+} \\
\alpha_{1}^{-} F_{1}+\alpha_{2}^{-} F_{2}=\bar{F}_{x}^{-}-\bar{F}_{x}=\beta^{-}
\end{array}\right.
$$

The solution is as follows:

$$
\begin{aligned}
& \left\{\begin{array}{l}
F_{1}=b_{1}^{-} \beta^{-}+b_{1}^{+} \beta^{+} \\
F_{2}=b_{2}^{-} \beta^{-}+b_{2}^{+} \beta^{+}
\end{array}\right. \\
& \left\{\begin{array}{l}
b_{2}^{-}=\frac{h_{x}^{2}}{\left(h_{x}^{-}+h_{x}\right)\left(h_{x}+h_{x}^{-}+h_{x}^{+}\right)} ; b_{2}^{+}=\frac{h_{x}^{2}}{\left(h_{x}^{+}+h_{x}\right)\left(h_{x}+h_{x}^{-}+h_{x}^{+}\right)} \\
b_{1}^{-}=-\frac{2 h_{x}^{+}+h_{x}}{h_{x}} b_{2}^{-} ; b_{1}^{+}=\frac{2 h_{x}^{-}+h_{x}}{h_{x}} b_{2}^{+} .
\end{array}\right.
\end{aligned}
$$

Fig. 18.11 Conservation of the average leakage over 3 adjacent cells. Definition of notations


Re-writing the weighting of the transverse leakage in terms of this expansion leads to:

$$
F_{x i}=\frac{1}{h_{x}} \int_{\frac{-h_{x}^{2}}{\frac{h_{x}}{2}}} f_{i}(x)\left[\bar{F}_{x}+F_{1} f_{1}(x)+F_{2} f_{2}(x)\right] d x \quad \text { hence: }\left\{\begin{array}{l}
F_{x 1}=\frac{F_{1}}{12} \\
F_{x 2}=\frac{F_{2}}{20}
\end{array}\right.
$$

### 18.5.3 AFEN Method

The Analytic Function Expansion Nodal (AFEN) ${ }^{9,10}$ method is one of the various methods which uses the eigenfunctions of the Laplace operator to build an intranodal form of the flux. Given the flux vector with two energy groups $\Phi(x, y)$ for a $2 D$ problem, a new quantity $\xi(x, y)$ is defined such that:

$$
\Phi(x, y) \equiv\binom{\Phi_{1}(x, y)}{\Phi_{2}(x, y)} \equiv \underbrace{\left(\begin{array}{cc}
\frac{\Sigma_{a, 2}-\lambda_{1} D_{2}}{\Sigma_{s, 1 \rightarrow 2}} & \frac{\Sigma_{a, 2}-\lambda_{2} D_{2}}{\Sigma_{s, 1 \rightarrow 2}} \\
1 & 1
\end{array}\right)}_{R}\binom{\xi_{1}(x, y)}{\xi_{2}(x, y)}
$$

The two-group diffusion equation without up-scattering in energy is written in matrix form as:

$$
-\left(\begin{array}{cc}
D_{1} & 0 \\
0 & D_{2}
\end{array}\right) \Delta \Phi+\left(\begin{array}{cc}
\Sigma_{a, 1}+\Sigma_{s, 1 \rightarrow 2}-\frac{\nu \Sigma_{f, 1}}{k_{e f f}} & -\frac{\nu \Sigma_{f, 1}}{k_{e f f}} \\
-\Sigma_{s, 1 \rightarrow 2} & \Sigma_{a, 2}
\end{array}\right) \Phi=0
$$

The $A F E N$ method consists in finding $\xi_{g}(x, y)$ as:

$$
\begin{aligned}
\xi_{g}(x, y)= & A_{g, 0}+A_{g, 1} \operatorname{sh}\left(\kappa_{g} x\right)+A_{g, 2} \operatorname{ch}\left(\kappa_{g} x\right)+A_{g, 3} \operatorname{sh}\left(\kappa_{g} y\right)+A_{g, 4} \operatorname{ch}\left(\kappa_{g} y\right) \\
& +B_{g, 1} \operatorname{sh}\left(\frac{\kappa_{g}}{\sqrt{2}} x\right) \operatorname{sh}\left(\frac{\kappa_{g}}{\sqrt{2}} y\right)+B_{g, 2} \operatorname{sh}\left(\frac{\kappa_{g}}{\sqrt{2}} x\right) \operatorname{ch}\left(\frac{\kappa_{g}}{\sqrt{2}} y\right) \\
& +B_{g, 3} \operatorname{ch}\left(\frac{\kappa_{g}}{\sqrt{2}} x\right) \operatorname{sh}\left(\frac{\kappa_{g}}{\sqrt{2}} y\right)+B_{g, 4} \operatorname{ch}\left(\frac{\kappa_{g}}{\sqrt{2}} x\right) \operatorname{ch}\left(\frac{\kappa_{g}}{\sqrt{2}} y\right)
\end{aligned}
$$

where each term (save for the first) is solution of the following equation for each computational cell:

[^371]$$
\Delta \xi_{g}(x, y)-\lambda_{g} \xi_{g}(x, y)=0 \quad g=1 \text { or } 2
$$
with $\kappa_{g}=\sqrt{\lambda_{g}}$. The constant value $A_{g, 0}$ is introduced to ensure that the neutron balance is guaranteed in each cell and disappears when the $k_{\text {eff }}$ converges. The nine coefficients for each cell are determined by expressing the average flux in the cell, the interface flux and the four fluxes at the vertices of the cell. The coupling between the cells is ensured via the neutron balance of the cell and the continuity of the four interface currents and the flux at the four corners of the cell. With currents on the left and right interfaces in $x\left(J_{g, x^{-}}, J_{g, x^{+}}\right)$for surface $A_{x}$ (resp. below and above in $y\left(J_{g, y^{-}}, J_{g, y^{+}}\right)$for $\left.A_{y}\right)$, the balance equation of the cell is written as:
\[

\left\{$$
\begin{array}{l}
\frac{J_{1, x^{-}}-J_{1, x^{+}}}{A_{x}}+\frac{J_{1, y^{-}}-J_{1, y^{+}}}{A_{y}}+\left(\Sigma_{a, 1}+\Sigma_{s, 1 \rightarrow 2}\right) \Phi_{1}=\frac{\nu \Sigma_{f, 1} \Phi_{1}+\nu \Sigma_{f, 2} \Phi_{2}}{k_{e f f}} \\
\frac{J_{2, x^{-}}-J_{2, x^{+}}}{A_{x}}+\frac{J_{2, y^{-}}-J_{2, y^{+}}}{A_{y}}+\Sigma_{a, 2} \Phi_{2}=\Sigma_{s, 1 \rightarrow 2} \Phi_{1}
\end{array}
$$\right.
\]

### 18.6 Finite Element Method

(Advances Nuclear Science and Technology Vol. 8, 1975, p. 173; Bathe 1982; Grandini 1986; Huebner 1975, p. 253; Lewis and Ward 1991; Logan 1986; Marchuk and Agochkov 1985; Oden 1972; Strang and Fix 1973; Zienkiewicz 1973)

The Finite Elements Method (FEM) was first developed in structural mechanical analysis. It is without doubt one of the numerical methods which has an extensive literature. Nowadays, it is one of the methods most widely employed by physicists of every branch. Reactor physics is no exception (Duderstadt and Hamilton 1976, p. 563). The finite element method stems from aeronautics with A. Hrennikoff (circa 1941) on the modeling of the rigidity of a structure of square cross section, represented by a bundle of coupled elementary rods (Grandini 1986, p. 2; Logan 1986, p. 2). In 1943, the German mathematician David Courant proposed an original numerical approach for the computation of mechanical stress using a Rayleigh-Ritz variational method (Huebner 1975, p. 9). The term "finite element method" was coined by R. W. Clough (1960). ${ }^{11}$ The goal of the finite element method is to approximate the behavior of unknown functions by a projection on known functions, then by integration over a mesh, to set up a linear system of equations consisting of coefficients of the functions. This is very similar to the nodal methods. The finite element methods are not restricted to the diffusion equation and have been applied to transport methods [an application of finite element methods to transport is given in (Mathematical aspects of FEM 1974,

[^372]p. 89) and in), ${ }^{12}$ although it is in diffusion that it has been most prevalent. For example, in $l D$, on a segment of length $\ell$ where the flux is zero at the boundaries:
$$
-D \Delta \Phi(x)+\Sigma_{a} \Phi(x)=\frac{\nu \Sigma_{f}}{k_{e f f}} \Phi(x)+S(x)
$$

For one energy group, the $\left(-D \Delta+\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right)$ [] operator is self-adjoint. This is no longer the case in multi-group. The flux is projected on a set of functions:
$\Phi(x)=\sum_{j=1}^{n} \varphi_{j} f_{j}(x)$ where the $f_{j}(x)$ verify the boundary conditions of the reactor.
This expression is substituted in the diffusion equation and the following is obtained:

$$
-D\left(\sum_{j=1}^{n} \varphi_{j} \frac{d^{2} f_{j}(x)}{d x^{2}}\right)+\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right)\left(\sum_{j=1}^{n} \varphi_{j} f_{j}(x)\right)=S(x)
$$

The Galerkin method (Fletcher 1984; Lewis and Ward 1991, p. 15; Marchuk and Agochkov 1985, p. 43; Grandini 1986, p. 315; Strang and Fix 1973, p. 116), consists in projecting the differential equation on each function $f_{i}$ with a scalar product defined as:

$$
\left\langle f_{i}, f_{j}\right\rangle \equiv \int_{x=0}^{x=\ell} f_{i}(x) f_{j}(x) d x
$$

This is equivalent to multiplying each term in the equation by $f_{i}(x)$ and integrating the resulting equations on $[0, \ell]$. The moment of the equations is obtained:

$$
-D\left(\sum_{j=1}^{n} \varphi_{j}\left\langle f_{i}, \frac{d^{2} f_{j}}{d x^{2}}\right\rangle\right)+\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right)\left(\sum_{j=1}^{n} \varphi_{j}\left\langle f_{i}, f_{j}\right\rangle\right)=\left(f_{i}, S\right)
$$

In similar fashion to the principles explained in the spherical harmonics expansion method for the transport equation, the functions $f_{i}(x)$ are chosen such that they are orthogonal. This simplifies the equations:
$-D\left(\sum_{j=1}^{n} \varphi_{j}\left\langle f_{i}, \frac{d^{2} f_{j}}{d x^{2}}\right\rangle\right)+\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right) \varphi_{i}=\left\langle f_{i}, S\right\rangle \forall i \quad$ if: $\left\langle f_{i}, f_{j}\right\rangle \equiv \int_{x=0}^{x=\ell} f_{i}(x) f_{j}(x) d x=\delta_{i j}$
A system consisting of $n$ linear equations in the $\varphi_{i}$ coefficients is obtained. The system is expressed in matrix form as:

[^373]\[

$$
\begin{aligned}
& -D \Delta_{i, j} \varphi_{j}+\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right) M_{i, j} \varphi_{j}=\mathrm{S}_{\mathrm{i}} \\
& \text { with: } \varphi=\left(\begin{array}{c}
\varphi_{1} \\
\vdots \\
\varphi_{i} \\
\vdots \\
\varphi_{n}
\end{array}\right), \quad \mathrm{S}=\left(\begin{array}{c}
\left\langle f_{1}, S\right\rangle \\
\vdots \\
\left\langle f_{i}, S\right\rangle \\
\vdots \\
\left\langle f_{n}, S\right\rangle
\end{array}\right) \text {, } \\
& \left.\Delta=\left(\begin{array}{ccc}
\left\langle f_{1}, \frac{d^{2} f_{1}}{d x^{2}}\right\rangle & \cdots\left\langle f_{1}, \frac{d^{2} f_{j}}{d x^{2}}\right\rangle & \cdots\left\langle f_{1}, \frac{d^{2} f_{n}}{d x^{2}}\right\rangle \\
\vdots \\
\left\langle f_{i}, \frac{d^{2} f_{1}}{d x^{2}}\right\rangle & \cdots\left\langle f_{i}, \frac{d^{2} f_{j}}{d x^{2}}\right\rangle & \cdots\left\langle f_{i}, \frac{d^{2} f_{n}}{d x^{2}}\right\rangle \\
\vdots \\
\left\langle f_{n}, \frac{d^{2} f_{1}}{d x^{2}}\right\rangle & \cdots\left\langle f_{n}, \frac{d^{2} f_{j}}{d x^{2}}\right\rangle \cdots\left\langle f_{n}, \frac{d^{2} f_{n}}{d x^{2}}\right\rangle
\end{array}\right) M=\left(\begin{array}{c}
\left\langle f_{1}, f_{1}\right\rangle \cdots\left\langle f_{1}, f_{j}\right\rangle \cdots\left\langle f_{1}, f_{n}\right\rangle \\
\vdots \\
\left\langle f_{i}, f_{1}\right\rangle \\
\vdots \\
\left\langle f_{n}, f_{1}\right\rangle
\end{array}\right)\left\langle f_{i}, f_{j}\right\rangle \cdots\left\langle f_{n}, f_{j}\right\rangle \cdots\left\langle f_{n}, f_{n}\right\rangle\right)
\end{aligned}
$$
\]

If the functions are orthogonal, the matrix $M$ simplifies into the identity matrix. The matrices are calculated only once, and if they are well conditioned, an iterative scheme can be used to solve the linear system. The existence of the Laplace operator $\Delta$ assumes that the functions $f_{j}$ can be derived twice, thereby restricting the choice of the functions to be used for the flux for strong variations. This problem may be alleviated by using a variational method. In the example above, this can be expressed by multiplying the diffusion equation by a function, and integrating over the volume of the reactor:

$$
-\int_{0}^{\ell} d x f(x) D \Delta \Phi(x)+\int_{0}^{\ell} d x f(x) \Sigma_{a} \Phi(x)=\int_{0}^{\ell} d x f(x) \frac{\nu \Sigma_{f}}{k_{e f f}} \Phi(x)+\int_{0}^{\ell} d x f(x) S(x)
$$

Integrating the first term by parts leads to:

$$
\int_{0}^{\ell} d x f(x) D \Delta \Phi(x)=\left[f(x) D \frac{d \Phi(x)}{d x}\right]_{0}^{\ell}-\int_{0}^{\ell} d x \frac{d f(x)}{d x} D \frac{d \Phi(x)}{d x}
$$

If a function $f(x)$ is chosen such that the boundary conditions are verified (i.e., it is worth zero at the limits of the reactor in our example), the first term of the previous equation cancels out. Hence, the following is obtained:

Weak formulation of the diffusion equation:

$$
\begin{align*}
\int_{0}^{\ell} d x \frac{d f(x)}{d x} D \frac{d \Phi(x)}{d x} & +\int_{0}^{\ell} d x f(x)\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right) \Phi(x)
\end{aligned} \begin{aligned}
& \equiv\left\langle\frac{d f(x)}{d x}, D \frac{d \Phi(x)}{d x}\right\rangle \\
+ & \left\langle f(x),\left(\Sigma_{a}-\frac{\nu \Sigma_{f}}{k_{e f f}}\right) \Phi(x)\right\rangle \tag{18.7}
\end{align*}
$$

This expression is called the weak formulation of the diffusion equation. This is because there exist functions that will verify the integral equation (known as the functional, which was described in Chap. 9), but without verifying the boundary conditions at all points of the interface. In multi-group, the group-by-group flux is expanded on the same basis functions $f_{j}$ :

$$
\Phi_{g}(x)=\sum_{j=1}^{n} \varphi_{j, g} f_{j}(x)
$$

The weak formulation is written for each group $g$ and each index $i$ :

$$
\begin{aligned}
& \sum_{g^{\prime}=1}^{G}\left\{\left\langle\frac{d f_{i}}{d x}, D_{g, g^{\prime}} \sum_{j=1}^{G} \varphi_{j, g^{\prime}} \frac{d f_{j}}{d x}\right\rangle+\left\langle f_{i},\left(\Sigma_{t, g, g^{\prime}}-\Sigma_{t, g, g^{\prime}}-\frac{\chi_{g} \nu \Sigma_{f, g^{\prime}}}{k_{e f f}}\right) \sum_{j=1}^{n} \varphi_{j, g^{\prime}} f_{j}\right\rangle\right\} \\
& \quad=\left\langle f_{i}, S_{g}(x)\right\rangle
\end{aligned}
$$

Mathematically, it can be proven that a function $\Phi(x)$ verifying the boundary conditions and the weak form of the equation for any function $f(x)$ verifying the boundary conditions (for which the integrals exist), is a solution of the problem. The advantage of this variational method is that the functions $f(x)$ need only be differentiable once and not twice as for the initial approach. This extends the domain of the projection functions to piecewise linear functions for example.

The numerical analysts developed myriads of finite elements more or less wellsuited to the type of problem at hand. Huebner (1975, p. 257) discusses the Helmholtz equation with tetrahedral elements with four nodes while (Advances Nuclear Science and Technology Vol. 8, 1975, p. 229) gives examples considering control rods with bilinear elements that are rectangular or even triangular close to the boundaries.

### 18.7 Variational Methods

### 18.7.1 Principle

Variational methods were applied first in astrophysics thanks to the works of V. Kourganoff ${ }^{13}$ in 1949, then in particle transport through the works of V.S. Vladimirov ${ }^{14}$ who truly developed the theoretical background. They are very similar to the finite element methods. In France, the initial works on this subject date from the 1960 s, ${ }^{15}$ under the guidance of J.L. Lions. The idea consists in formulating a functional resulting from the integration of surface and volume terms from the diffusion equation on a given volume $V=\cup V_{i}$ :

$$
f(\Phi, \vec{J}) \equiv \sum_{V_{i} \in V} \int_{V_{i}}\left(D(\overrightarrow{\operatorname{grad}} \Phi)^{2}+\Sigma_{a} \Phi^{2}-2 \Phi S\right) d V+2 \int_{\partial V_{i}} \Phi \vec{J} . \vec{n} d \Gamma
$$

Since the flux verifies the diffusion equation with fission source $S$ :

[^374]
V.S. Vladimirov source: Teoreticheskaya i Matematicheskaya Physika 94, 1 (1993), photograph unknown
${ }^{15}$ Hoan Nguyen-Ngoc: Résolution variationnelle des Equations de diffusion multigroupe indé pendantes du temps [Variational resolution of time-independent multi-group diffusion equations], thesis presented to the University of Paris (1965).
$$
-\operatorname{div}(\overrightarrow{\operatorname{grad}} \Phi)+\Sigma_{a} \Phi=S
$$

The goal is to obtain a positive functional to be minimized so as to be amenable to the mathematical tools associated with such problems. Introducing the current as a Lagrange multiplier in the surface term and expanding the flux and the current on basis functions, we obtain variational nodal methods. The flux is expanded as:

$$
\Phi(\vec{r})=\sum_{l} \varphi_{l} f_{l}(\vec{r})
$$

Where $f_{l}(\vec{r})$ are polynomials in the column vector $f(\vec{r})$ that verifies the orthogonality condition:

$$
\int_{V_{i}} f(\vec{r}) f^{T}(\vec{r}) d V=V_{i} I \quad \text { where } I \text { is the unit vector }
$$

The flux is thus expressed as $\Phi(\vec{r})=f^{T}(\vec{r}) \times \varphi$ where $\varphi$ is the coefficient column vector and $\times$ represents the matrix-vector products. Similarly, the following relation can be written: $\vec{J}(\vec{r}) \cdot \vec{n}=h^{T}(\vec{r}) \times j$. Orthogonal polynomials are chosen preferentially as a basis of trial functions $h(\vec{r})$ such that:

$$
\int_{\partial V} h(\vec{r}) h^{T}(\vec{r}) d \Gamma=I
$$

The flux can also be projected on this basis for points belonging to the surface $\overrightarrow{r_{\Gamma}} \in \partial V:$

$$
\Phi\left(\overrightarrow{r_{\Gamma}}\right)=h^{T}\left(\overrightarrow{r_{\Gamma}}\right) \times \psi
$$

The coefficients $j$ and $\psi$ in the basis are given by:

$$
j=\int_{\partial V} h(\vec{r}) \vec{J}(\vec{r}) \cdot \vec{n} d \Gamma \text { and } \psi=\int_{\partial V} h(\vec{r}) \Phi(\vec{r}) d \Gamma
$$

Where, by substitution of $\Phi(\vec{r})$ in the equation for $\psi$ leads to:

$$
\psi=M^{T} \varphi \text { with }: M^{T}=\int_{\partial V} f(\vec{r}) h^{T}(\vec{r}) d \Gamma
$$

Functions $f$ are a complete basis of polynomials of order $p$ (for instance, the first $p$ Legendre polynomials in $l D$ ) if it is of dimension $(p+1)(p+2) / 2$ in $2 D$ Cartesian geometry and $4 p+1$ for $h$ to account for the four edges of the cell. If $p=p$, an exact projection of $\Phi(\vec{r})$ on the surfaces of the cell is obtained. The functional is transformed to include $j$ and $\psi$ by substitution of the expansions of $\Phi(\vec{r})$ and $\vec{J}(\vec{r})$ :

$$
f(\varphi, j)=\sum_{V_{i} \in V}\left[\varphi_{V_{i}}^{T} A_{V_{i}} \varphi_{V_{i}}-2 \varphi_{V_{i}}^{T} \int_{V_{i}} f S d V+2 \varphi_{V_{i}}^{T} M j\right]
$$

with: $A_{V_{i}}=\int_{V_{i}}\left(D(\overrightarrow{\text { gradf } f})\left(\overrightarrow{\text { grad }^{\prime}} f^{T}\right)\right) d V+\Sigma_{a} V_{i} I$. Modeling may be refined either by increasing spatial discretization while keeping the same set of trial functions, or by increasing the polynomial order of the trial functions.

### 18.7.2 Accounting for Boundary Conditions

Given that the boundary conditions of a cell with surface $\Gamma=\Gamma_{n} \cup \Gamma_{r}$ :

$$
\left\{\begin{array}{l}
\Phi\left(\overrightarrow{r_{s}}\right)=0 \text { for } \overrightarrow{r_{s}} \in \Gamma_{n} \quad \text { Zero }- \text { flux condition } \\
D\left(\overrightarrow{r_{s}}\right) \frac{\partial \Phi}{\partial n}\left(\overrightarrow{r_{s}}\right)+\gamma \Phi\left(\overrightarrow{r_{s}}\right)=0 \text { for } \overrightarrow{r_{s}} \in \Gamma_{r} \text { Robin condition }
\end{array}\right.
$$

Starting from the Kourganoff functional, similar to that of Vladimirov:

$$
f(\Phi) \equiv \int_{V}\left(\operatorname{divD} \overrightarrow{\operatorname{grad}} \Phi-\Sigma_{a} \Phi^{2}+2 \Phi S\right) d^{3} r
$$

From the Ostrogradski theorem, the first term of the integral is written as:

$$
\begin{aligned}
\int_{V} d i v D \overrightarrow{\operatorname{grad}} \Phi d^{3} r & =-\int_{V} D(\overrightarrow{\operatorname{grad} \Phi} \Phi)^{2} d^{3} r+\int_{\Gamma} \Phi D \vec{n} \cdot \overrightarrow{\operatorname{grad}} \Phi d^{2} r \\
& =-\int_{V} D(\overrightarrow{\operatorname{grad}} \Phi)^{2} d^{3} r+\underbrace{\int_{\Gamma_{n}} \Phi D \vec{n} \cdot \overrightarrow{\operatorname{grad}} \Phi d^{2} r}_{0}+\underbrace{}_{\Gamma_{r}} \gamma \Phi^{2} d^{2} r
\end{aligned}
$$

The flux that turns the system into a stationary one is next sought:

$$
\delta f(\Phi)=\int_{V}\left(-2 d i v D \overrightarrow{\operatorname{grad}} \Phi \overrightarrow{\operatorname{grad}} \delta \Phi-2 \Sigma_{a} \Phi \delta \Phi+2 \delta \Phi S\right) d^{3} r-2 \int_{\Gamma_{r}} \gamma \Phi \delta \Phi d^{2} r=0
$$

For any function $\Psi$ (Fig. 18.12):

$$
\begin{equation*}
\int_{V}\left(d i v D \overrightarrow{\operatorname{grad}} \Phi \overrightarrow{\operatorname{grad}} \Psi+\Sigma_{a} \Phi \Psi-2 \Psi S\right) d^{3} r+\int_{\Gamma_{r}} \gamma \Phi \Psi d^{2} r=0 \tag{18.8}
\end{equation*}
$$

Fig. 18.12 Finite element with eight vertices

which can be handled by means of a classical approach with finite elements, using a parallelepiped with eight vertices as the basis element:

$$
\Phi(x, y, z)=\sum_{i, j, k}^{8} \varphi_{i j k} f_{i j k}(x, y, z)
$$

with: $f_{i j k}(x, y, z)=\sum_{l=1}^{2} \sum_{m=1}^{2} \sum_{n=1}^{2} f_{l m n}^{i j k} l^{l-1} y^{m-1} z^{n-1}$ where the coefficients $f_{l m n}^{i j k}$ are calculated such that the function is worth 1 at the vertex $i, j, k$ and 0 elsewhere.

The stationary side of the functional is expressed by projecting each term of Equation (18.8) on the basis functions:

$$
\left\langle f_{i j k}, S\right\rangle=\sum_{i^{\prime}, j^{\prime}, k^{\prime}}\left[\left\langle\overrightarrow{\operatorname{grad}_{i j k}} f_{i \overrightarrow{g r a d}} f_{i^{\prime} j^{\prime} k^{\prime}}\right\rangle-\left\langle f_{i j k}, \Sigma_{a} f_{i^{\prime} j^{\prime} k^{\prime}}\right\rangle+\left\langle f_{i j k}, \gamma f_{i^{\prime} j^{\prime} k^{\prime}}\right\rangle_{\Gamma_{r}}\right] \varphi_{i^{\prime} j^{\prime} k^{\prime}}
$$

where the scalar product is defined classically for an elementary volume $V_{i}$ :

$$
\left\langle f_{i j k}, g\right\rangle=\int_{V_{i}} f_{i j k} g d^{3} r \text { and }\left\langle f_{i j k}, g\right\rangle_{\Gamma_{r}}=\int_{\Gamma_{i} \cap \Gamma_{r}} f_{i j k} g d^{2} r
$$

The linear system obtained is solved using classical matrix methods. The problem is generalized to multi-group settings by iterating on the groups starting from the group of fast-energy neutrons.

### 18.8 Calculation of Control Rods

(Meghreblian and Holmes 1960, p. 721) for the theoretical aspects
Most reactors have a reactivity control system based on the insertion of rods of solid absorbers. These rods, of various shapes (cylindrical pins in PWR, crossshaped control rods in BWR, slabs in certain experimental reactors, etc.), are


Fig. 18.13 Control rod placement for a 900 MWe PWR
often-but not always-located above the core. This ensures that in emergency situations the rods may be inserted by means of gravity. For PWR, they are placed above the assemblies of the active core (Fig. 18.13). These rods result in marked heterogeneity due to their radial position in the core, which breaks up the symmetry of the core pattern, or to their axial insertion in the core, when their absorbing nature disrupts the flux distribution.

### 18.8.1 Physical Effect of Rods

(Physics and Material Problems of Reactor Control Rods 1964)
A rod is composed of neutrons-absorbing materials (for example, steel or a mixture of silver-indium-cadmium or boron carbide $B_{4} C$ ), which exerts complex effects on the flux (Fig. 18.14).

Perpendicular to the control rod, thermal flux tends practically to 0 (Glasstone and Edlund 1972, p. 317; Lamarsh and Baratta p. 349; Glasstone and Sesonske


Fig. 18.14 Effect of a rod on thermal flux
1994, p. 304; Lewins 1978, p. 42). If flux is normalized such that the integral is conserved (e.g. normalization to a given power), it tends to increase at the periphery of the core, thereby increasing leakage. This effect also exists in the axial direction (Stacey 2001, p. 80), and combination of these two phenomena (absorption and leakage) contribute to the decrease in $k_{\text {eff. }}$. Accurate determination of the rod worth is a key element in reactor safety evaluation [anti-reactivity margins, (Kerkar and Paulin 2008, p. 43)], which is further complicated by the fact that inserted rods produce a shadowing effect, with all types of reactor. This shadowing effect results in the rod worth of a group of rods being lower than the sum of the individual rod worths.

### 18.8.2 Rod Worth: Perturbation Analysis

Historically, control rod calculation was formalized in France during the development of the $U N G G$ design at the end of the 1950s. Initially, a global perturbation approach was considered since control rods exert long-range action in reactors with graphite moderators due to the size of the migration area. Certain theoretical aspects of perturbation theory will be recalled for the sake of our analysis (Duderstadt and Hamilton 1976, p. 223). In one-group theory (Kahan and Gauzit 1957), the diffusion equation describing the reactor is written as:

$$
\begin{equation*}
\text { Flux equation of state: } \frac{1}{v} \frac{\partial \Phi}{\partial t}=D \Delta \Phi+\left(k_{\infty}-1\right) \Sigma_{a} \Phi \tag{18.9}
\end{equation*}
$$

in which we will include the $H$ operator: $\frac{\partial \Phi}{\partial t}=H[\Phi]$. The exponential matrix approach, described in the reactor fuel cycle chapter, enables this differential system to be solved (if in $3 D$ ):

$$
\Phi(t)=e^{H t} \Phi(0)
$$

The vector $\Phi(0)$ may be expanded on the basis of eigenvectors of $H$ :

$$
\Phi(0)=\sum_{i=0}^{N} \varphi_{i} \Phi_{i}
$$

This leads to: $\Phi(t)=\sum_{i=0}^{N} e^{\lambda_{i} t} \quad \varphi_{i} \Phi_{i}$ with $H\left[\Phi_{i}\right]=\lambda_{i} \Phi_{i}$
The eigenvalues are ordered such that the $\lambda_{0}$ eigenvalue associated with the fundamental mode, denoted as $\Phi_{0}$, is real and is larger than the real part of all the other eigenvalues (Planchard 1995). Let $H^{*}$ be the adjoint matrix (the transpose of the conjugate matrix). If $H$ has real components, $H^{*}=H^{t}$, and the eigenvalues of $H^{*}$ are the same as those of $H$. Moreover, the eigenvectors of $H$ and that of $H^{*}$ are orthogonal two-by-two when the eigenvalue of the two vectors are different. If $H^{*}$ $=H$, the matrix is self-adjoint (or Hermitian), which is the case in one-group theory. In this particular situation, the eigenvalues are all real and the eigenvectors are orthogonal, two at a time. If a perturbation $\Delta H$ is applied to the matrix, the flux is perturbed and is worth $\Phi_{0}^{\prime}$, which verifies the following:

$$
(H+\delta H)\left[\Phi_{0}^{\prime}\right]=\left(\lambda_{0}+\delta \lambda_{0}\right) \Phi_{0}^{\prime}
$$

The adjoint flux verifies: $H^{*}\left[\Phi_{0}^{*}\right]=\lambda_{0} \Phi_{0}^{*}$. Defining the $<>$ operator as the integration over the total volume of the reactor, the perturbed equation can be written from the perturbed equation:

$$
<\Phi_{0}^{*}(H+\delta H) \Phi_{0}^{\prime}>=<\Phi_{0}^{*}\left(\lambda_{0}+\delta \lambda_{0}\right) \Phi_{0}^{\prime}>=\left(\lambda_{0}+\delta \lambda_{0}\right)<\Phi_{0}^{*} \Phi_{0}^{\prime}>
$$

Similarly, $<\Phi_{0}^{\prime}\left(H^{*}\right) \Phi_{0}^{*}>=<\Phi_{0}^{\prime} \lambda_{0} \Phi_{0}^{*}>=\lambda_{0}<\Phi_{0}^{\prime} \Phi_{0}^{*}>=\lambda_{0}<\Phi_{0}^{*} \Phi_{0}^{\prime}>$
By expanding $<\Phi_{0}^{*}(H+\delta H) \Phi_{0}^{\prime}>=<\Phi_{0}^{*} H \Phi_{0}^{\prime}>+<\Phi_{0}^{*} \delta H \Phi_{0}^{\prime}>$
hence the importance of the results of the perturbation of the eigenvalue to the first order:

$$
\delta \lambda_{0}=\frac{<\Phi_{0}^{*} \delta H \Phi_{0}^{\prime}>}{<\Phi_{0}^{*} \Phi_{0}^{\prime}>}
$$

This result nevertheless requires knowledge of the perturbed fundamental mode $\Phi_{0}^{\prime}$, necessitating a critical calculation, which is of limited interest since the calculation of $\Phi_{0}^{\prime}$ gives $\lambda_{0}^{\prime}=\lambda_{0}+\delta \lambda_{0}$. Assuming that $\Phi_{0}^{\prime} \approx \Phi_{0}$, the equation may be restricted to:

$$
\delta \lambda_{0}=\frac{<\Phi_{0}^{*} \delta H \Phi_{0}>}{<\Phi_{0}^{*} \Phi_{0}>}
$$

For one energy group in which $\Phi_{0}^{*}=\Phi_{0}$ rigorously, the formula is obtained by weighting by the squared value of the flux. Within Eq. (18.9), the perturbation of the matrix by an absorber is expressed as:

$$
\delta H=v \delta\left[\left(k_{\infty}-1\right) \Sigma_{a}\right]
$$

where: $\delta \lambda_{0}=\frac{\int_{V} v \delta\left[\left(k_{\infty}-1\right) \Sigma_{a}\right] \Phi_{0} \Phi_{0}^{\prime} d V}{\int_{V} \Phi_{0} \Phi_{0}^{\prime} d V}$
Starting from a critical state $\left(\lambda_{0}=0\right)$, the reactivity of the perturbed state $\rho=\delta k_{\text {eff }} / k_{\text {eff }}$ can be approximated by:

$$
\begin{aligned}
& \frac{1}{v} \frac{\partial \Phi^{\prime}}{\partial t}=\frac{\lambda_{0}^{\prime}}{v} \Phi^{\prime}=\frac{\delta \lambda_{0}}{v} \Phi^{\prime}=D \Delta \Phi^{\prime}+\left(k_{\infty}^{\prime}-1\right) \Sigma_{a} \Phi^{\prime}=-D B^{\prime 2} \Phi^{\prime}+\left(k_{\infty}^{\prime}-1\right) \Sigma_{a} \Phi^{\prime} \\
& \text { Hence: } \rho=\frac{\delta \lambda_{0}}{v k_{\infty}^{\prime} \Sigma_{a}}
\end{aligned}
$$

If a long-range absorber is inserted in a $U N G G$ core, the following can be written for the whole pile:

$$
k_{\infty}^{\prime} \Sigma_{a}^{\prime} \approx k_{\infty} \Sigma_{a}=c s t \quad \text { on the pile } \quad \Rightarrow \delta\left(k_{\infty} \Sigma_{a}\right)=0
$$

where:

$$
\begin{equation*}
\text { Rod worth in one-group theory: } \rho=-\frac{\int_{V} \delta \Sigma_{a} \Phi_{0} \Phi_{0}^{\prime} d V}{k_{\infty} \Sigma_{a} \int_{V} \Phi_{0} \Phi_{0}^{\prime} d V} \tag{18.10}
\end{equation*}
$$

The reader should note that this formula is valid only for one energy group, which is an acceptable approximation for highly thermal reactors with graphite moderator where the rods have a long-range effect. However, it is not suitable for water reactors in which the influence of a rod is limited to two or three assemblies. Further, the reactor must be close to critical state. Nevertheless, this formula extends the application of using a flux-squared weight for more significant perturbations. Experimental studies conducted during physics tests cycles of the EDF2 reactor in 1965 showed that the formula yielded more precise results for a rod at the center of the core (compared with the flux-squared formula), and more particularly, with a constant error. Allowance can be made for the eccentric position of a rod in the core by slightly modifying the formula to include a non-constant $k_{\infty} \Sigma_{a}$ over the entire core:

$$
\rho=-\frac{\int_{V} \delta\left[\left(k_{\infty}-1\right) \Sigma_{a}\right] \Phi_{0} \Phi_{0}^{\prime} d V}{\int_{V} k_{\infty} \Sigma_{a} \Phi_{0} \Phi_{0}^{\prime} d V}
$$

### 18.8.3 Measuring Rod Efficiency in PWR

(Techniques de mesure des barres de commande (Measuring techniques for control rods 1976; Murray 1954, p. 319)

As seen earlier, in diffusion theory, the interfaces are not correctly computed, all the more so in the presence of highly absorbent materials. Since precise computation of rods is crucial for safety analysis it is of great interest. For each loading, preliminary theoretical studies and a series of measurements are carried out at zero power before the reactor start-up. These procedures are essential to validate the conformity of the loading pattern with respect to both safety and design criteria. Amongst other procedures, rod efficiency is measured and compared to the theoretical computed value, and the discrepancy between the two must not exceed $10 \%$ in absolute value (this is a design criterion). This value is used to determine the antireactivity available within rod banks for use in maneuvers during the reactor operation such as load monitoring, or, in the event of an incident, an emergency stop. The measuring procedure currently employed is the dilution-swapping method, which comprises two steps:

- Determination of the worth of the reference rod bank (the power regulation bank) by dilution: with core criticality being maintained, the rod bank is inserted from the "all rods out" position to the lower position, and the boron concentration is diluted to compensate for this insertion. The variations in reactivity, which depend on the position of the rod bank, are used to determine the differential and integral efficiency of the rod bank.
- Determination of the worth of the other rod banks by swapping: the previous bank is used as reference. The rod bank to be evaluated is inserted; core criticality is maintained by simultaneously extracting the reference rod bank. The position of the latter when the rod bank under measurement is completely inserted provides the efficiency value via the previous measurement by dilution.

While this technique enables highly precise measurement of rod bank efficiency, it is extremely time-consuming (completion of all measurements for a $900-\mathrm{MWe}$ reactor takes 12 to 14 h ), generates boron effluents, and can be a problem for effluent management. To overcome the various problems posed by the dilutionswapping method, a new technique for measuring the integral efficiency of rod banks was developed and successfully tested in the United States. The modus operandi of this method, known as Direct Rod Worth Measurement, consists in inserting the measured rod bank at maximum velocity from the higher to the lower
position, from the reactor slightly over-critical, before returning it to the higher position. This phase is repeated with the next rod bank. During insertion of the rod bank, the flux variations in the core are measured and stored by the external power chamber using a digital reactimeter. Using the post-processing program, the signal is post-processed to obtain the static integral efficiency of the rod bank. As for measurement by the dilution-swapping method, the general principles consist in using inverse kinetics computation to deduce the reactivity from the signal registered by an external flux detector. However, the physical phenomena occurring during the measurement are complex (flux redistribution, delayed-neutron effect). Under such conditions, the spatial and dynamics effects are of two types:

- The static spatial effect due to the change in the core environment resulting from insertion of the rod bank leads to immediate redistribution of prompt neutrons.
- The dynamic effect is due to changes in the spatial distribution of delayed neutrons, which is out of phase with that of the prompt flux.

The advantage of this method is that it is far faster. For example, for a 900 MWe reactor, the complete process takes less than 3 h . In addition, this method does not generate any boron effluent, leading to significant time savings, and thus increases the availability of the reactor. For fast neutron reactors, rod worths are measured in a different manner since it is not possible to use the method involving dilution of boron, which is absent from the primary circuit. The techniques can be classified into three categories, employing:

- analysis of neutron noise based on signal processing (coherence method, etc.);
- kinetic techniques based on sub-critical flux behavior over time (reactimeter, Carpenter method, etc.);
- statistical techniques based on sub-critical flux behavior (asymmetric source method, source multiplication method, ${ }^{16}$ etc.)


### 18.8.4 Calculation of Rod Efficiency

Accounting for the rod effect in a diffusion calculation consists in meshing the core such that one edge of the axial mesh is tangent to the edge of the rod. In this configuration, the mesh cells contain homogeneous materials, either with rod or without rod. This method is suitable only if the rod is fixed. In the case of motion of the rod, cells must be created on-the-fly as a time function. This procedure has numerical implications and can be costly if the core geometry is changed frequently, leading to the definition of a homogenized cross section for Partially

[^375]Rodded Medium ( $P R M$ ). The basic technique to define this cross section, $\Sigma_{\alpha}^{P R M}$, consists in volume-weighting the absorption cross section (resp. fission) in the presence of the media (Fig. 18.15) so as to conserve the reaction rates (Fig. 18.16):

Fig. 18.15 Rod inserted in an axial cell


Fig. 18.16 Visualization of an inserted rod


$$
\Sigma_{\alpha}^{P R M} \bar{\Phi} V_{t o t}=\Sigma_{\alpha}^{A} \bar{\Phi}_{A} V_{A}+\Sigma_{\alpha}^{B} \bar{\Phi}_{B} V_{B}
$$

Assuming the neutron flux as being equal in both zones of the partially rodded cell (given that there is only one calculation cell, the flux is a cell-averaged flux) and noting that the right cross-section of the homogenized assembly is the same as that of the homogenized rod, we have:

$$
\Sigma_{\alpha}^{P R M}=\frac{a \Sigma_{\alpha}^{A}+b \Sigma_{\alpha}^{B}}{a+b}
$$

However, this type of weighting raises homogenization problems. Although the cross sections of the cell are determined by an average weighted by the volume of the inserted rod in the mesh, the multiplication factor appears to vary with a "wavelike" structure when an absorbing rod is inserted in meshes with fixed cells. These oscillations are especially visible on analysis of the differential efficiency of the rod within the core, i.e. the derivative of the reactivity with respect to the axial position of the rod (Fig. 18.17).

These oscillations constitute a troublesome numerical artifact (highly localized increase in reactivity can occur on insertion of a rod) that worsens with coarser meshes. This oscillation, also called rod cusping, is even more apparent in kinetic cases in which a rod is inserted or removed, where all conditions conspire to cause numerical oscillations since the tip of the rod moves through a cell. The direct method for rod worth measurement, which uses pre-computed coefficients to postprocess measurements from external detectors, is sensitive to such oscillations due to the very principle of the inverse kinetics method. Oscillation problems in fact make up part of the wider field of methods associated with the homogenization process: since flux does not vary linearly with respect to the cross sections, neither does the homogenization process. The problem can be alleviated by using a weighting method that involves conservation of the reaction:


Fig. 18.17 Differential reactivity as a function of insertion step

$$
\Sigma_{g}^{P R M}=\frac{a \bar{\Phi}_{g}^{A} \Sigma_{\alpha_{g}}^{A}+b \bar{\Phi}_{g}^{B} \Sigma_{\alpha_{g}}^{B}}{a \Phi_{g}^{A}+b \Phi_{g}^{B}}
$$

The mean flux $\bar{\Phi}_{g}^{B}$ is approximated as the average flux in the non-rodded part of cell $k$ and cell $k+1$ (lower cell). The mean flux $\bar{\Phi}_{g}^{A}$ is approximated as the average of the flux in the partially rodded cell $k$ and cell $k+1$ (upper cell):

$$
\Phi_{g}^{A}=\frac{a \bar{\Phi}_{g}^{k^{A}}+h_{k-1} \Phi_{g}^{k-1}}{a+h_{k-1}} \text { and } \Phi_{g}^{B}=\frac{b \bar{\Phi}_{g}^{k^{B}}+h_{k+1} \Phi_{g}^{k+1}}{b+h_{k+1}}
$$

As with all weighting methods using the flux and volume, the problem consists in determining the mean flux in all zones, both rodded and unrodded. For the sake of simplicity, the flux in the rodded zone of the cell may be approximated by assuming that it is equal to the flux in the upper cell, while the flux in the unrodded zone of the cell is taken to be that of the lower cell. This "extrapolation" technique smoothens the phenomenon without any physical background. Han-Sem Joo proposed ${ }^{17}$ that the intra-nodal shape of the flux in the partially rodded cell be computed starting from a reference situation in which the exact flux is determined by making the rod extremity coincide with the cell edge (as close as possible to the configuration being studied, Fig. 18.18). The intra-nodal form of the flux is considered accurate and is applied to the partially rodded cell. This method shifts the shape of the flux obtained in the reference case to the partially rodded case. This postulates that the physical problem is not modified axially over a distance smaller than the cell height: it is assumed that the axial shape of the flux does not vary significantly around the rod


Fig. 18.18 Joo translation method: the intra-nodal form computed for a reference situation is translated to the rodded problem

[^376]tip. The flux in the partially rodded cell is thus known-at least approximatelyand the flux-volume weight can be applied to compute the homogenization of neutron quantities. This approach is linked to nodal methods where the shape of the flux is postulated, and is very costly given the need for calculation in the reference situation, either on the fly or by adding a calculation step when the rod moves through a cell edge in order to preserve the intra-nodal form.

The spectral index method is also based on cross-section homogenization by flux and volume weighting. It seeks to determine the neutron flux in a rodded zone and non-rodded zone using the spectral index, i.e. the ratio of the fast flux to the thermal flux. The spectral index is known in advance since it is determined by the type of fuel assembly in an infinite lattice for instance. The thermal flux can be deduced from the fast flux throughout the whole core:

$$
\bar{\Phi}^{\text {Therm } . A}=\frac{\Phi_{\text {Therm }}^{\text {Assemb } . A}}{\Phi_{\text {Fast }}^{\text {Assemb.A }}} \bar{\Phi}_{\text {core }}^{\text {Fast }} \quad \text { and } \quad \bar{\Phi}^{\text {Therm } . B}=\frac{\Phi_{\text {Therm }}^{\text {Assemb. } B}}{\Phi_{\text {Fast }}^{\text {Assemb } . B}} \bar{\Phi}_{\text {core }}^{\text {Fast }}
$$

The spectral index of the assembly is first computed, then the partially rodded cell is determined and the volume fraction calculated. The fast flux is determined by a flux-volume approximation of some sort, and the thermal flux is then determined using the above equations. Finally, the cross section is homogenized using a classical flux-volume approach. This method is warranted since the fast flux in a PWR core presents less significant local variation than the thermal flux, given that the rod is generally a thermal absorber.

### 18.8.5 Analytical Decomposition of the Rodded Domain

Another approach consists in computing the average fast and thermal flux in the rodded and unrodded zones of the cell by analytical solution of the diffusion equation for two energy groups in the partially rodded cell. This method provides an analytical means of dealing with domain decomposition since it can be generalized by locally meshing the rodded cell and applying the boundary conditions at the surface of the sub-domain. For the sake of simplicity, this analytical resolution will be done in $1 D$. This approximation can be bypassed by applying the radial leakage in the diffusion equation. Nonetheless, it is justified by the fact that the firstorder effect of the rod acts principally on the axial thermal flux. In the present case, this equation is reduced to one dimension, and with an additional term for neutron leakage $\Sigma_{\text {leakage }}$, and with $\Sigma_{t, 1}=\Sigma_{a, 1}+\Sigma_{r}$, it is written for zone $A$ as follows:

$$
\left\{\begin{array}{l}
-D_{1} \frac{\partial^{2} \Phi_{1}(z)}{\partial z^{2}}+\left(\Sigma_{t, 1}+\Sigma_{\text {leakage }_{1}}\right) \Phi_{1}(z)=\frac{1}{k_{\text {eff }}}\left(\nu \Sigma_{f 1} \Phi_{1}(z)+\nu \Sigma_{f 2} \Phi_{2}(z)\right) \\
-D_{2} \frac{\partial^{2} \Phi_{2}(z)}{\partial z^{2}}+\left(\Sigma_{t, 2}+\Sigma_{\text {leakage }_{2}}\right) \Phi_{2}(z)=\Sigma_{r} \Phi_{1}(z)
\end{array}\right.
$$

The resolution of this equation, using techniques described in the chapter on the homogeneous reactor, leads to a fourth-degree equation for each zone without leakage:

$$
\Delta \Delta \Phi_{2}(x)+\underbrace{\left[\frac{\nu \Sigma_{f 1}}{D_{1} k_{e f f}}-\frac{D_{1} \Sigma_{t, 2}+D_{2} \Sigma_{t, 1}}{D_{1} D_{2}}\right]}_{b} \Delta \Phi_{2}(x)+\underbrace{\frac{\Sigma_{t, 1} \Sigma_{t, 2}}{D_{1} D_{2}}\left(1-\frac{k_{\infty}}{k_{e f f}}\right)}_{c} \Phi_{2}(x)=0
$$

The sign of coefficient $c$ depends on the $k_{\infty} / k_{\text {eff }}$ ratio and coefficient $b$ may be either positive (for $k_{e f f}<\frac{\nu \Sigma_{f 1}}{\Sigma_{t, 1}+\frac{D_{1}}{D_{2}} \Sigma_{t, 2}}$ ) or negative (for $k_{e f f}>\frac{\nu \Sigma_{f 1}}{\Sigma_{t, 1}+\frac{D_{1}}{D_{2}} \Sigma_{t, 2}}$ ).

Let $\lambda^{2}$ and $\mu^{2}$ be the roots of the fourth-degree equation valid for both zones:

$$
\begin{gathered}
x^{4}+b \cdot x^{2}+c=0 \\
\text { Let: }\left\{\begin{array}{l}
\lambda^{2}=\frac{-b+\sqrt{\Delta}}{2} \\
\mu^{2}=\frac{-b-\sqrt{\Delta}}{2}
\end{array} \text { with } \Delta \equiv b^{2}-4 c\right.
\end{gathered}
$$

For cases that follow the physics of the problem: $D_{1} \approx 2 D_{2}$ and $\Sigma_{t, 2} \approx 2 \Sigma_{t, 2}$. The only case where $\Delta$ can be negative is that where $k_{\text {eff }}$ is large (and larger than c), but increasing $k_{\text {eff }}$ leads to an increase in $b^{2}$. Ultimately, the determinant remains positive. The sign of $\lambda^{2}$ is driven by the sign of $c$ only if $b$ is positive. The situation may be summarized as follows:

$$
\left\{\begin{array}{lll}
\text { if } b>0 & \text { and } c>0 & \Rightarrow \lambda^{2}<0 \\
\text { if } b>0 & \text { and } \mu^{2}<0 \\
\text { if } b<0 & \text { and } c>0 & \Rightarrow \lambda^{2}>0 \\
\text { and } \mu^{2}<0 \\
\text { if } b<0 & \Rightarrow \lambda^{2}>0 & \text { and } \mu^{2}>0 \\
\text { if } c<0 & \Rightarrow \lambda^{2}>0 & \text { and } \mu^{2}<0
\end{array}\right.
$$

By means of reductio ad absurdum, ${ }^{18}$ it can be shown that the first solution is physically impossible. Indeed, $\lambda^{2}<0$ if $b>0$ and $k_{\infty}<k_{e f f}$, hence:

$$
\frac{\nu \Sigma_{f 1} \Sigma_{t, 2}+\nu \Sigma_{f 2} \Sigma_{r}}{\Sigma_{t, 1} \Sigma_{t, 2}}<k_{e f f}
$$

Let us further assume: $\frac{\nu \Sigma_{f 1}}{k_{e f f}}+\frac{\nu \Sigma_{f 2} \Sigma_{r}}{k_{\text {eff }} \Sigma_{t, 2}}<\Sigma_{t, 1}$
Then: $\frac{\nu \Sigma_{f 1}}{k_{e f f}}<\Sigma_{t, 1}$ and $\frac{\Sigma_{t, 1}}{D_{1}}-\frac{\nu \Sigma_{f 1}}{k_{\text {eff }} D_{1}}>0$
which means that $b \equiv \frac{\nu \Sigma_{f 1}}{D_{1} k_{e f f}}-\frac{D_{1} \Sigma_{t, 2}+D_{2} \Sigma_{t, 1}}{D_{1} D_{2}}<0$

[^377]Table 18.1 Eigenfunctions of intra-nodal fluxes

| Configuration | Eigenfunctions of the flux |
| :--- | :--- |
| $\lambda^{2}<0$ and $\mu^{2}<0, b>0$ and $c>0$, | $\left\{\begin{array}{l}f=\cos , f^{*}=\sin \\ g=\cos , g^{*}=\sin \end{array}\right.$ |
| that is $k_{\infty}<k_{\text {eff }}$ |  |
| Physically impossible | $\left\{\begin{array}{l}f=c h, f^{*}=\operatorname{sh} \\ g=\cos , g^{*}=\sin \end{array}\right.$ |
| $\lambda^{2}>0$ and $\mu^{2}<0$, whatever the sign of $b, c<0$, <br> that is $k_{\infty}>k_{\text {eff }}$ | $\left\{\begin{array}{l}f=c h, f^{*}=\operatorname{sh} \\ g=c h, g^{*}=s h\end{array}\right.$ |
| $\lambda^{2}>0$ and $\mu^{2}>0, b<0$ and $c>0$, |  |
| that is $k_{\infty}<k_{\text {eff }}$ |  |

This assertion is inconsistent with the initial hypothesis (Table 18.1).
The flux is written as:

$$
\left\{\begin{array}{l}
\Phi_{1}(z)=\alpha \frac{\left(\Sigma_{t, 2}-D_{2} \lambda^{2}\right)}{\Sigma_{r}} f(\lambda z)+\beta \frac{\left(\Sigma_{t, 2}-D_{2} \lambda^{2}\right)}{\Sigma_{r}} f^{*}(\lambda z)+ \\
\gamma \frac{\left(\Sigma_{t, 2}-D_{2} \mu^{2}\right)}{\Sigma_{r}} g(\mu z)+\delta \frac{\left(\Sigma_{t, 2}-D_{2} \mu^{2}\right)}{\Sigma_{r}} g^{*}(\mu z) \\
\Phi_{2}(z)=\alpha f(\lambda z)+\beta f^{*}(\lambda z)+\gamma g(\mu z)+\delta g^{*}(\mu z)
\end{array}\right.
$$

In the presence of leakage, the total cross section $\Sigma_{t}$ is only replaced by $\left(\Sigma_{t}+\Sigma_{\text {leakage }}\right)$ where $\Sigma_{\text {leakage }}=D B_{g}^{2}$. The situation where an unrodded medium admits a flux solution as $s h$ and $c h$ is theoretically possible in the presence of significant leakage, even though this would normally be expected with a rodded medium. Finally, there are 8 unknowns to be computed ( $\alpha, \beta, \gamma, \delta$ for $A$ and $B$ ) in order to determine the analytical flux in the two zones. The boundary and edge conditions for the partially rodded cell must still be determined in order to solve the equations. The system can be solved either by imposing the currents at the edges of the mesh or by imposing the flux. If the choice is to set the currents at the boundaries, there are 4 equations for boundary conditions: 2 equations per group and per zone. 4 further equations must be imposed. For this purpose, the 4 equations corresponding to the flux and current continuity between the rodded and unrodded media are written for each of the two energy groups. A linear system of 8 equations with 8 unknowns is obtained. It can be solved using a numerical algorithm [e.g. Gauss-Jordan for example, (Varga 1962; Gastinel 1966, p. 88)]. However, the choice of the conditions to be applied is of crucial importance. In fact, the 4 equations with respect to the continuity of flux and current at the interface between the two zones are fixed such that the physics of the problem is preserved at the rod/fuel interface. The possible choice on the 4 remaining equations is made from the 8 possible boundary conditions (flux and current in zone $A$ in the fast and thermal groups, flux and current in zone $B$ in the fast and thermal groups), i.e. $C_{8}^{4}=70$ possibilities. A single choice on the conditions set for the flux leads to an imposed value of $k_{\text {eff }}^{\text {cell }}$, with the analytical flux consistent with the edges by construction, at the expense of preservation of the flux shape in the cell. On the other hand, the choice on the conditions set for the current leads to an inconsistent flux shape for the

Fig. 18.19 Search for the root of the critical determinant (TexeraudMassaud calculations, 2008)

Determinant

same value of $k_{\text {eff }}^{\text {cell }}$. The addition of a ninth condition would allow the calculation of a $k_{\text {eff }}^{\text {cell }}$ value different from $k_{\text {eff }}^{\text {core }}$. The search for the roots ${ }^{19}$ of the critical $8 \times 8$ determinant corresponding to the boundary conditions enables determination of $k_{\text {eff }}^{\text {core }}$ for the fundamental mode, bound by the values of $k_{\infty}^{A}$ and $k_{\infty}^{B}$ of the rodded and unrodded media respectively.

$$
k_{\infty}^{A}=\frac{\nu \Sigma_{f 1}^{A} \cdot \Sigma_{a 2}^{A}+\nu \Sigma_{f 2}^{A} \cdot \Sigma_{r}^{A}}{\Sigma_{a 2}^{A} \cdot \Sigma_{t, 1}^{A}} k_{\infty}^{B}=\frac{\nu \Sigma_{f 1}^{B} \cdot \Sigma_{a 2}^{B}+\nu \Sigma_{f 2}^{B} \cdot \Sigma_{r}^{B}}{\Sigma_{a 2}^{B} \cdot \Sigma_{t, 1}^{B}}
$$

Note that for geometries with high leakage, although it is not particularly intuitive, $k_{\text {eff }}^{\text {core }}$ is not bounded by the values $k_{\infty}^{A}$ and $k_{\infty}^{B}$. In a configuration with two zones and low leakage, two roots are obtained, the smallest of which is retained (in the example, 1.14844 and 1.48512, Fig. 18.19), since it corresponds to the largest eigenvalue $\lambda$ of the diffusion operator, $\Delta \Phi=\lambda\left(\nu \Sigma_{f}-\Sigma_{a}\right) \Phi / D$. After analysis, the most precise method consists in imposing the calculated $k_{\text {eff }}^{\text {core }}$ on the whole core. In an iterative approach to compute $k_{\text {eff }}^{\text {core }}$, the value from the previous iteration is chosen. The analytical solutions are sought by imposing the fast flux and the fast current on the edges of the meshes, which are influenced less by the presence of the rod. Knowing the shape of the flux in the partially rodded cell leads to a homogenization process that significantly diminishes ( $50-80 \%$ ) the oscillations, but without completely removing them. In neutron kinetics, the analytical decomposition of the flux for a rodded domain disregards the transient term; while this makes less justifiable, it is acceptable for small cells, which is generally the case for industrial core meshes. A domain decomposition technique would probably be more efficient than over-meshing the rodded cell but would be more onerous in terms of calculation time, especially for kinetics.

[^378]
### 18.9 Instrumentation Considerations

The historical internal instrumentation of PWR is based on the RIC system (Reactor In-core Control), which consists of mobile fission chambers inserted from the bottom of the reactor vessel. These chambers are stored outside the core, and are placed in an immersion sleeve located in the central instrumentation tube of $17 \times 17$ assemblies of the core during monthly flux measurements (flux maps). Once inserted into the core, the fission chambers measure the activity enabling measurement to be made of the neutron flux after reconstruction.

### 18.9.1 Modeling with Trace Quantities

The response of the detector is computed with a calculation code and compared to measurements. The simplest solution consists in introducing the notion of "trace quantities" in the calculation of neutron libraries with the transport theory. A very small amount of the isotope present in the detector is added to the moderator of the guide tube (where it reacts with the flux) without modeling the detector itself or the sleeve in which it is located. This very small quantity is warranted because of the need to avoid permanent parasitical captures in the assembly, since the detector remains inside for some ten hours. For mobile fission chambers (FC), the trace consists of a thinlayer deposit of uranium 235, which by fission, generates fission products that ionize a gas. The electrons produced by this ionization are measured. Hence, the detector is not modeled explicitly with this trace technique. Moreover, the sleeve located within the instrumentation tube is not modeled either. Non-instrumented assemblies do not have a sleeve and their central instrumentation tube is filled with moderator. Instrumented assemblies, however, have a sleeve throughout the entire cycle. Since the sleeve takes the place of a given volume of moderator, there is a difference in neutron behavior that is not detected by the trace quantity instrumentation.

### 18.9.2 Modeling of the EPR Instrumentation: The KTM Model

The instrumentation of the new EPR (European Pressurized Reactor) has been redesigned to provide greater reliability and speed during its use. To avoid penetration from the bottom of the reactor vessel, the internal instrumentation is designed to be inserted from the top of the reactor. In the interests of redundancy, two new types of instrumentation have been introduced (Fig. 18.20):

- Aeroball sensors where the working principle consists in blowing in a column of vanadium ball bearings in an instrumentation tube. The term aeroball sensor is used. The vanadium is activated in the core. The column of ball bearings is removed


Fig. 18.20 Example of an aeroball sensor (left) and a collectron (right)
to measure activity when outside the core. The advantage of this system is its speed of use: each measurement takes only a few minutes vs. hours for FC measurements.

- Collectron canes comprising a cobalt or rhodium detector. The detection principle is as for FC. Activation of the detector isotope is measured continuously. This is the main improvement over FC: collectrons remain inside the core and inside certain assemblies they are placed in a collectron cane with 6 axial detectors at different heights.

As with the sleeves for the FC, the collectron canes and aeroball sensors occupy the place of a small amount of moderator inside the instrumentation tube. Moreover, in an EPR assembly, there may be an additional fuel ( 265 vs . 264 for the other reactors), since the canes are not placed in the central tube but in the guide tubes for the rods (which implies that an instrumented assembly cannot be rodded).

During safety analysis of the instrumentation system, the question of the impact of the instrumentation canes was posed in two parts:

- What is the cumulative impact of the presence of the instrumentation cane on the assembly power, given that its position is not symmetric? It is logical to assume


| A1 | dêtecteur |
| :--- | :--- |
| A2 | fourreau |
| A3 | support |
| A4 | modérateur |
| A5 | doigt de gant |
| B1 à | cabbles |
| B5 |  |



Fig. 18.21 Example of the lower collectron (D1) and that directly above (D6) which is influenced by the cables of the lower collectrons
that an assembly with permanent instrumentation during an operation cycle will have modified neutron behavior. This cumulative effect causes a deviation in composition compared to a similar assembly without instrumentation. This is called a historical effect and acts on the cross sections. Furthermore, if the instrumentation is removed, the moderator that replaces the volume in the instrumentation tube leads to a local overpower situation due to overmoderation. This is an instantaneous effect on the cross sections. In the case of collectron canes, axial absorption is affected according to the height considered (six cables at the top, one at the bottom, see Fig. 18.21).

- What is the impact on the fine power structure for an assembly that has been "decollectronized", a neologism meaning that the collectron cane (or aeroball sensor) has been removed for a new cycle? This question is all the more disturbing since an overpower effect is anticipated due to the introduction of a large volume of water on removal of the cane, resulting in local overmoderation. As with cross sections, there is a historical and instantaneous effect on the fine power structure.

To deal with this complex subject, in 2011, Denis Kerdraon, ${ }^{20}$ Jérôme Texeraud $^{21}$ and Serge Marguet ${ }^{22}$ proposed the KTM model (comprising the initials

[^379]of their name as well as an allusion to the famous Austrian motorcycle brand). This model is based on explicit representation of the instrumentation. The underlying principle is to model the instrumentation as accurately as possible in the infinite lattice calculation in transport theory. First, a depletion calculation of the assembly is carried out without the instrumentation. At the same time, several other depletion calculations are carried out for the various instrumented assembly configurations (with aeroball sensor only, with collectron cane, and aeroball sensor). It should be noted that a collectron cane alone is not possible: all assemblies with a collectron cane also have an aeroball sensor. The numerical implementation in COCCINELLE consists in defining these new media as "shades" of the reference non-instrumented medium. When the non-instrumented assembly is loaded into the code (these media are said to be "primary"), the shades, which will be required according to the loading pattern and the current position of the instrumentations, are automatically loaded. Hence, a "neutron shade" is a slight modification of the base medium. Using a judicious naming convention for the neutron media, the shades can be determined automatically (Fig. 18.22).

The core of the EPR reactor is constituted of assemblies without instrumentation, assemblies with an aeroball sensor and assemblies containing a double instrumentation system with collectron/aeroball sensors. Due to the fuel management by third or quarter fractioning, an assembly may be instrumented or not according to the different "scenarios". For instance, the following is possible:

"C" denotes Collectron, "A" denotes Aeroball and" denotes no instrumentation
Hence, by considering each slab within an independent assembly (composed of four slabs), the instrumentation history of the slab can be created. For the scenario in the above assembly:

[^380]

Fig. 18.22 Scheme of the instrumentation positions in the EPR

- The upper left slab sees the following scenario ( $\left.{ }^{\prime} \mathrm{A}^{\prime}, \mathrm{A}^{\prime}, \mathrm{A}^{\prime}\right)$ :

- The upper right slab sees the scenario (' ',' ',' '):
$\square$
$\square$
$\square$
- The lower left slab sees the scenario (' ',' ',' '):
$\square$
$\square$
$\square$
- The lower right slab sees the scenario (' $\mathrm{C}^{\prime},{ }^{\prime}{ }^{\prime},{ }^{\prime}$ '):


The KTM model has two fundamental postulates: one concerning cross sections and the other concerning fine power structures.

### 18.9.2.1 Cross Sections in the KTM Model

The KTM model assumes that the cross sections in a slab depend solely on the burnup level and the shade of the medium. This means that the historical aspect of the slab is not explicitly taken into account. This historical effect is assumed to be accounted for by the current burn-up level since any change in the instrumentation of a slab will modify its burn-up. Let us take for example the upper left slab described previously: $\tau_{1}$ is the burn-up level at the end of the first cycle, $\tau_{2}$ that of the second cycle and $\tau_{3}$ that of current cycle ( $\tau_{1}<\tau_{2}<\tau_{3}$ ):

$$
\Sigma\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3}\right)=\Sigma\left(\text { medium }, \tau_{3},{ }^{\prime} \mathrm{A}^{\prime}\right) \equiv \Sigma_{K T M}\left(\text { shade }_{\mathrm{A}^{\prime}}, \tau_{3}\right)
$$

This means that the cross sections depend on the medium, the local burn-up $\tau_{3}$ of the slab, the current instrumentation (here Aeroball $=\mathrm{A}$ ) and also on the instrumentation history. In the example, the slab in the upper left sees Aeroball instrumentation in all cycles. More examples illustrating the method are given below. For a slab with no instrumentation in the current cycle, the primary medium cross sections are used (Fig. 18.23):

$$
\begin{gathered}
\Sigma\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime}{ }^{\prime}, \tau_{3}\right)=\Sigma\left(\text { medium }, \tau_{3},{ }^{\prime} '\right) \equiv \Sigma_{K T M}\left(\text { medium }, \tau_{3}\right) \\
\Sigma\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime}{ }^{\prime}, \tau_{2},{ }^{\prime} \mathrm{C}^{\prime}, \mathrm{C}^{\prime}, \tau_{3}\right)=\Sigma\left(\text { medium }, \tau_{3},{ }^{\prime} \mathrm{C}^{\prime}\right) \equiv \Sigma_{K T M}\left(\text { shade } \mathrm{C}^{\prime}, \tau_{3}\right)
\end{gathered}
$$

### 18.9.2.2 Fine Power Structures in the KTM Model

Fine power structures (FPS), erring on the side of conservatism, correspond to a disadvantageous history (with respect to the hotspot). In fact, the aim of the KTM model is to obtain a hotspot in the core that is at least equal to one obtained in reality. Computation of all the historical effects for all possible instrumentation is extremely costly in terms of calculation time and memory footprint. Assuming 4 cycles with 3 possible instrumentations ( $\mathrm{A}^{\prime}, \mathrm{C}^{\prime} \mathrm{C}^{\prime \prime \prime}$ ), $3^{4}=81$ combinations are obtained. This is multiplied by the number of branch calculations for the depletion. The resulting neutron physics library would be huge and the calculation time of the library would be incompatible with operational constraints.

The fine power structure depends on:


Fig. 18.23 Principle of KTM for cross sections

- The moderation seen by a slab, according to the presence or absence of instrumentation. A slab without instrumentation is more moderated than an instrumented one. This is the instantaneous effect.
- The isotopic composition of the pins in the slab. The isotopic composition depends of the past history of the slab, especially its instrumentation state. This historical effect is simply the integral of the instantaneous effect over time.

Fine calculations for scenarios show that the fine power structure depends more or less on the instrumentation history of the previous cycles, especially if the history is close (the immediately previous cycle is more influential than older cycles). This effect is called a fade-out effect, which is one of the elements of the historical effects. The FPS to be used for power factorization is present in the identifier of the
first cycle state with a branch calculation corresponding to the current state identifier and the extraction burn-up on transition between instrumented and non-instrumented states (the "decollectronization" neologism is used to express the removal of the cane). For instance, for a slab undergoing a second cycle and no longer instrumented with an aeroball sensor as of $10,000 \mathrm{MWd} /$ ton, the code uses the FPS in an aeroball medium with a branch state corresponding to extraction at $10,000 \mathrm{MWd} /$ ton. If this burn-up is not specifically present in the library (which is tabulated for a few extraction burn-ups only), a linear interpolation is carried out between the two available extraction burn-ups (Fig. 18.24).

Given that not all possible situations of change have been considered, a penalized scenario is set up using the real history of the assembly slab. The library generator manages only a single change for the scenarios of each slab. For example, the FPS for 4-cycle scenarios ( $\mathrm{A}^{\prime \prime}, \mathrm{A}^{\prime},{ }^{\prime \prime}$, ) and ( $\mathrm{C}^{\prime},{ }^{\prime \prime}, \prime, \prime$ ) will be available in a library while that of the scenarios ( $\mathrm{A}^{\prime},{ }^{\prime \prime}, \mathrm{C}^{\prime}, \mathrm{C}^{\prime} \mathrm{C}^{\prime}$ ) and ( $\mathrm{A}^{\prime},{ }^{\prime \prime}, \mathrm{A}^{\prime},^{\prime \prime}$ ) will not. It will thus be

Fig. 18.24 "Sliding" decollectronization: branch calculations are carried out by varying the extraction burn-up for decollectronization



Fig. 18.25 Comparison of fine structures before and after instrumentation: aeroball (left), and collectron (right). Power loss appears around $5 \%$ less with the collectron than with the aeroball
necessary to substitute scenarios with more changes by those that are more disadvantageous with respect to the hotspot.

The various preliminary studies showed collectron instrumentation to be more disadvantageous at slab level. Figure 18.25 shows the discrepancies between FPS for a non-instrumented assembly and the same assembly instrumented at position $(14 ; 4)$. There is a net power loss of $-5 \%$. This situation, cumulated over a complete cycle, leads to under-irradiation of the pins surrounding the instrumentation in an explicit representation calculation. When this instrumentation is removed, the in-flow of moderator in place of the sleeve generates a local power surge since the surrounding pins are less depleted. The collectron case is more disadvantageous if the slab has seen a collectron cane during the previous cycles (historical effect).

From this observation, the disadvantageous scenarios are determined in the following way

- If the slab has been through only one cycle, then the disadvantageous scenario is the same as the real one;

$$
\pi\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1}\right) \equiv \pi_{K T M}\left(\text { shade }^{A_{A}}, \tau_{1}\right)
$$

- If the cycles of the slab have included no instances of instrumentation or only one, then the disadvantageous scenario is the same as the real scenario; $\pi\left(\right.$ medium, $\left.{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3}, \mathrm{~A}^{\prime}, \tau_{4}\right)=\pi\left(\right.$ medium, $\left.{ }^{\prime} \mathrm{A}^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\right.$ shade $\left._{\mathrm{A}^{\prime}}, \tau_{4}\right)$ $\pi\left(\right.$ medium $\left.,{ }^{\prime} \mathrm{C}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{3},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right)=\pi\left(\right.$ medium $\left.,{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\right.$ shade $\left.^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right)$
- If all the cycles of the slab have been through only one change, the disadvantageous scenario:
- is equal to the real scenario if it consists of an instrumented/non-instrumented change;

$$
\begin{aligned}
& \pi\left(\text { medium },{ }^{\prime} \mathrm{C}^{\prime}, \tau_{1},{ }^{\prime}{ }^{\prime}, \tau_{2},{ }^{\prime \prime}, \tau_{3},{ }^{\prime \prime}{ }^{\prime}, \tau_{4}\right)=\pi\left(\text { medium },{ }^{\prime} \mathrm{C}^{\prime}, \tau_{1},{ }^{\prime \prime}{ }^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\text { shade }^{\prime}{ }^{\mathbf{C}},{ }^{\prime}, \tau_{1},{ }^{\prime \prime}, \tau_{4}\right) \\
& \pi\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime \prime}, \tau_{3},{ }^{\prime \prime}, \tau_{4}\right)=\pi\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\text { shade }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime \prime}, \tau_{4}\right)
\end{aligned}
$$

- corresponds to the presence of a collectron at each cycle if the change is between an aeroball and a collectron (the only change not computed by GAB);
$\pi\left(\right.$ medium $\left.,{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{3},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right)<\pi\left(\right.$ medium $\left.,{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\right.$ shade $\left.{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right)$
$\pi\left(\right.$ medium $\left.,{ }^{\prime} \mathrm{C}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{4}\right)<\pi\left(\right.$ medium $\left.,{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\right.$ shade $\left.^{\prime}{ }^{\mathrm{C}}, \tau^{\prime}, \tau_{4}\right)$
- if there has been more than one change between the different cycles, the more disadvantageous instrumentation seen by the various cycles is determined and the scenario is completed as follows:
- If the current cycle of the slab is not instrumented, then, from cycle 1 to the last instrumented cycle, it is completed with the disadvantageous instrumentation "seen" by the slab;

$$
\begin{aligned}
& \pi\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3},{ }^{\prime \prime}, \tau_{4}\right)<\pi\left(\text { medium },{ }^{\prime} \mathrm{C}^{\prime}, \tau_{3}{ }^{\prime}{ }^{\prime}{ }^{\prime}, \tau_{4}\right) \\
& \times \equiv \pi_{K T M}\left(\text { shade }{ }^{\prime} \mathrm{C}^{\prime}, \tau_{3},{ }^{\prime \prime}, \tau_{4}\right) \pi\left(\text { medium, }{ }^{\prime} \mathrm{A}^{\prime}, \tau_{1},{ }^{\prime \prime}, \tau_{2},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3},{ }^{\prime}, \tau_{4}\right) \\
& \times \pi\left(\text { medium },{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3},{ }^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\text { shade }{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3},{ }^{\prime}{ }^{\prime}, \tau_{4}\right)
\end{aligned}
$$

- If the current cycle of the slab is instrumented, then the scenario is completed from the first instrumented cycle to the last cycle by the most disadvantageous instrumentation "seen" by the slab.

$$
\begin{aligned}
& \pi\left(\text { medium, }{ }^{\prime \prime}, \tau_{1},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{2},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{3},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{4}\right)<\pi\left(\text { medium },^{\prime \prime}, \tau_{1},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right) \\
& \times \equiv \pi_{K T M}\left(\text { medium, } \tau_{1},{ }^{\prime} \mathrm{C}^{\prime}, \tau_{4}\right) \pi\left(\text { medium,' ' }, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{2},{ }^{\prime \prime}, \tau_{3},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{4}\right) \\
& \times<\pi\left(\text { medium, },{ }^{\prime \prime}, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{4}\right) \equiv \pi_{K T M}\left(\text { medium }, \tau_{1},{ }^{\prime} \mathrm{A}^{\prime}, \tau_{4}\right)
\end{aligned}
$$

In conclusion, a disadvantageous algorithm is available and guarantees that the fine power structure applied to the homogeneous power of the assembly slab will produce a hotspot factor higher than the actual scenario: the result is thus conservative with respect to safety considerations. In practice, two "shaded" media which see only one extraction or insertion of instrumentation need to be computed and two burn-ups are thus required: the extraction/insertion burn-up and the current one.

The KTM model is one of the neutron physics models that take historical effects into account.

## Conclusion

We have just reviewed the main theoretical models that allow us to grasp reactor physics. I understand that it might be very frustrating to reach the end of a textbook on reactor physics without ever having encountered a nice picture of a reactor. However, the technological aspects are very significant in the nuclear reactor field and deserve to be examined on more than just a page or two of general conceptsconcepts that can, today, be easily found on the internet in any case. This is why I have deliberately omitted from this textbook any feature that is too technological to only concentrate on the physics which is, in itself, a very wide subject. A future textbook on the physics of nuclear accidents will be more appropriate for discussing reactors and technology.

What can we conclude from roughly 70 years of reactor physics? As often, the best comes with the worst. Some reactors have operated for 40 years without any problems whereas, in its very first year of operation, an accident at the TMI-2 reactor caused damage beyond repair. Regardless of the ongoing technological progress, our understanding of the underlying physics is improving: better knowledge of cross sections and materials behaviour under irradiation, allowing for probabilistic safety studies and human factors, and so on. Neutron physics is also advancing, for example, in the field of analytical and numerical resolution of the transport equation and more precise homogenization theories. I am also referring to novel domain decomposition techniques, where each zone of the reactor can be considered using a separate and suitable model, both in terms of meshing or resolution method of the Boltzmann equation. ${ }^{1}$ The tens of scientific journals devoted to nuclear engineering is a testament to the renewal of the field as well. How far we have come since Fermi's pile went critical in 1942! It is hard to imagine how the theoretical physicists of the time managed to perform this feat so quickly

[^381]after the discovery of fission. Calculation codes have also progressed at a stupendous pace as evidenced by the boxes of old punch cards still found sometimes in the depths of archives.

Although they are not the perfect solution to the problems of a world which is continuously more demanding in energy, fission reactors need to be placed amongst the various energy production means, and there will probably be many more of them in the next 50 years. The current problems of our time are appropriate: oil becoming rarer, global warming ... However, the task will not be very easy unless reactor physicists continue to set higher safety standards. Other reactors will be designed and built: breeder reactors to deal with the gradual use-up of natural fissile material, and safer reactors such as those studied in the Generation IV studies for innovative designs. The life of the current French fleet is coming to an end and the situation is very much the same around the world. This will require an aggressive building policy from operators in the future. The renewal of the French fleet by the French-German EPR in France and Finland is a good illustration of that. The position of the United States on the renewal of its fleet and that of emerging countries on nuclear power will most definitely be instrumental in the short term.

What are the next challenges in reactor physics? We would suggest the resolution of a $3 D$ core with fine deterministic transport, in "one go" killing the two-steps procedure (spectral assembly codes followed by 3D-space-time reactor codes), the Holy Grail of neutron transport-which may very well become possible sooner than one might think, if the technology of massively parallel computing improves at the same pace as information technology did during the past 40 years. Or we could say depletion, or even kinetic, Monte Carlo calculations applied to exact geometries. Furthermore, "on-line" codes continuously fed by experimental measurements, which are already known to be faster than real-time processes, should also be investigated, but for now, are still seldom employed by operators. These codes could be used along with new data assimilation methods that can be essential for the fitting phase. Also, a better operation of the instrumentation of present reactors or future instrumentation could lead to a more insightful "view" of the behaviour of the core. In the near future, it is likely that new computational schemes will abandon the classical two energy-group diffusion calculation approach substituted by methods using simplified transport but with multi-group. Multi-physics coupling of specialized codes will become more prevalent so that the physical modelling of phenomena becomes consistent, i.e., this means not having high-performing physics in one field being associated to too simplistic models in another-as for e.g. a $3 D$ neutron-kinetic model coupled with $1 D$ quasi-static thermal-mechanics. Another field of study will probably be the development of adjoint codes with high perturbation orders to finally obtain uncertainties not solely based on the renowned but controversial "engineer's judgment".
. . .until the avail of fusion?
Reactor physics still has some good days ahead!
Serge Marguet
Clamart, September 17, 2009

# Annex: Reactor Physics and Neutronic Codes at Electricité De France 

The end of this book seems a fitting moment, to paraphrase Stephen Hawking, for $a$ brief history of reactor physics and neutronic codes at Electrcité De France. At $E D F$, which was created by French nationalization legislation in 1946, a studies and research department was set up immediately (Picard 1987).

(EDF)
One of the first reference works on physics archived at the Documents Department et the Research and Studies Department $(D E R)$ in Clamart is this course report on Atomic Engineering compiled (hand-written !) in 1955 by the EDF Atomic Engineering "commando" team, B. Saïtcevsky, D. Gaussot et al: The design of an electricity-producing reactor using natural uranium with zirconium cladding, cooled by pressurized heavy water.

Pierre Ailleret, who graduated from the French Polytechnique School in 1918, was appointed as the first director (he remained with EDF until 1958), was unanimously recognized as "the most learned electrical engineer amongst us", in the words of Pierre Massé, who himself became director of Equipment in 1946 (Picard et al. 1985, p. 92). EDF was then a company of electrical and hydraulic engineers, and it was logical that the expertise of the newly formed R\&D called
$D E R$ should gravitate towards these two professional areas. Conventional thermal engineering was something of a poor relation, and was abandoned without compunction to the Production Department. When the CEA developed piles G1, G2 and $G 3$ to produce plutonium for military uses (Bonnet 1980) p. 111, Pierre Ailleret, who had been a member of the CEA scientific committee since 1950, while his own brother, General Ailleret, was the deputy head of the Military Applications Department of the $C E A$ (he oversaw the French tests in the Sahara), kept a close eye on the development of the industrial program, and took all necessary steps to ensure that an electricity production system would be installed at the G1 pile in Marcoule (agreement protocol of May 14, 1954).


Pierre Ailleret (1900-1996) is the craftsman of the development of the civil nuclear energy in France (EDF)

Pierre Guillaumat, then head of the $C E A$, was in favor of "handing over" to $E D F$ management of the nuclear facilities, despite bitter grievances among certain CEA members, led by Jules Horowitz, criticized what he saw as "nonsensical sharing" (Picard et al. 1985, p. 188).

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ÉLECTRICITÉ DE FRANCE
    DIRECTION
DES ETUDES ET RECHERCHES
PARIS, LE
12, PLACE DES 后TATS-UNIS
    TELL. : KL自BER 02-20
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The first address of the $D E R$ in a well-off district of Paris (letterhead of the time)
In 1955 the "Sous-Région d'Equipement Nucléaire 1" (Nuclear Equipment Sub-region 1) was set up under the direction of Jean-Pierre Roux (the term "subregion" in itself reflects the disdain for this business by the majority at $E D F$ ), which
in 1957 became the "Région d'Equipement Thermique Nucléaire" or Nuclear Equipment Region (RETN: viewpoints evolved rapidly!) in Clamart. Claude Bienvenu, one of the rare thermal engineers at $E D F$, and who himself would become director of the $D E R(R \& D)$, was appointed head of the affair on the $E D F$ side.

(EDF)
Claude Bienvenu (1927-2011) will be the first ever nuclear engineer of EDF. Bienvenu is graduate of the prestigious Polytechnique engineering school, engineer of Sup' aero in 1949. He enters the DER in 1951 when he is appointed head of the department studies in 1955. In 1960, he is named assistant director of the region of thermal and nuclear equipment $n^{\circ} 1$, then will manage in 1963 the RETN 2. He finishes his career as general inspector of EDF before retirement in 1992.

Following divergence in 1956, the demonstrator pile struggled to produce 5 MWe even though 6 MW were necessary to turn the cooling blowers injecting air into the reactor, thus giving a negative energy balance. However, technical feasibility was demonstrated and the construction of a power reactor in Chinon (on the river Loire) was considered.

Jules Horowitz, Director of Piles at the CEA and one of France's leading reactor physicists of his time, was convinced that the $C E A$ could manage such an industrial program by itself, with $E D F$ participation limited to steam production, since it was a fact that the public company did not have a single neutron physicist on its payroll.

(EDF)
REN1 was extremely proud of its three UNGG facilities, as this leaflet from May 1967 attests
However, $E D F$ did not see things this way and in the mixed $E D F-C E A$ teams, the $E D F$ turned their attentions primarily to the core, while the $C E A$ engineers were especially drawn to the steam generators! But $E D F$ imposed its own viewpoints and
the reactor in Chinon was dubbed EDF1 (60 MWe, divergence in 1962). It was followed by EDF2 (1964) and EDF3 (1966). In 1962, RETN was split into 3 sections: REN1 (Clamart) which took up residence opposite the $D E R$ (it had moved out of the Place des Etats-Unis in the 16th arrondissement of Paris, which was now too small), REN2 (in Tours, under the direction of Bienvenu) and a Department of General Nuclear Studies, which was a forerunner of the engineering section of the Equipment Department (Torres and Lefebvre 1996, p. 238).The Department was interested to Boris Saïtcevski (1926-), a researcher at $D E R$-Chatou who, having studied Atomic Engineering in 1955, was one of the very small group of in-house reactor physicists. Indeed, few $E D F$ engineers such as Denis Gaussot, who would go on to become director of SEPTEN, had been asked to follow the Atomic Engineering course in 1955. Saïtcevski was entrusted with all aspects of reactors and became the single point of contact with the CEA. He later became director of NERSA, the European company responsible for building and running the Superphénix.


Boris Saïtcevski, circa 1960, EDF

Acquisition of knowledge in the field was haphazard: $E D F$ engineers were assigned to $U N G G$ teams at the $C E A$ to follow the experimental MARIUS and CESAR programs. The "Documentation" Department in Chatou, like the US Central Intelligence Agency, had Russian documents translated, including the famous paper by Bondarenko method on cross sections (1964).

(EDF)
Construction of the test buildings in Chatou on the "Ile des Impressionistes" in October 1949. Chatou is one of the three historic R\&D sites, together with Clamart, and later, Les Renardières. Activities at the site today are concerned primarily with hydraulics and thermal hydraulics, with neutron physics being concentrated in Clamart.

Regarding computer codes, David Feingold (1929-), after completing his studies in mathematics at the Faculté des Sciences of Paris, was recruited in 1958 by the DER, which was then still located at the Place des Etats-Unis. He joined up with Jean Carteron, Jean Abadie and Gérard Deloux to carry out calculations on neutron scattering. These computations were performed on a Gamma computer weighing 4 tonnes(!) built by the Bull company and installed at the Place des Etats-Unis, pending the arrival of a future Gamma 60. This attempt to use French equipment by Bull ended in failure and the DER next turned to IBM equipment. Shortly afterwards, Feingold left for the United States where in 1959 he studied the emerging techniques of scientific computing at Columbia University, returning to the US in 1962 for 6 months under Prof. Richard Steven Varga ${ }^{2}$ to study neutron transport codes alongside Jean Abadie and computer specialist Philippe Larcher (1919-1986). Varga worked from 1954 until 1960 at the Bettis Atomic Power Laboratory of Westinghouse in Pittsburgh, where he developed numerical methods suited to the question of

[^382]eigenvalue problems for reactor criticality. He then taught at the Case Institute in Cleveland. In this way, it was in the United States that the first EDF 3D neutron transport code for diffusion theory was created, based on the Westinghouse methods! On his return, Feingold re-joined the Department of Mathematical Studies and New Related Applications in Clamart, and was in fact one of the first people to actually work at the site, which was still under construction. The first calculator installed at Clamart was a 7094 devoted solely to neutron physics, but the subsequent creation of the ERCA departments or the arrival of CDC 6600-6400, which were also used for calculations concerning electrical networks. From October 1962, he worked on the creation of a two-dimensional to group code with finite differences, incorporating Chebyshev acceleration and block over-relaxation, using principles based on (Varga 1962), and he communicated regularly with Varga. Together with P. Larcher, he finally produced the JANE code ( $3 D$ diffusion code using the finite-difference method, for four energy groups, 500 physical media cells, and 13,500 points in a square-lattice mesh), an ancient ancestor of the COCCINELLE code. Feingold became director of the Data Processing and Mathematical Studies Department, and he retired in 1990.


## (Courtesy Feingold)

David Feingold, seen here in 1979, was a pioneer in neutronic codes at EDF. He oversaw the incredible development of calculation power at the company's Clamart site.


Richard Varga (Public domain)

Thanks to this 1969 report, the main codes used at the time are remembered. The main reactor physics codes were MUDE for multigroup diffusion equation (1D), and ALCI and its derivative (MICALCI and MIALCI 3) for 2D multigroup diffusion. The Russian 26 -groups Bondarenko databank of cross sections was also available.


Modifications of the main neutronic codes used at EDF by E. Charasse, J. Martin et J.P. Pasquet, note EDF HZ0108 (1969). Every sketch was hand-made by the time! (The Marguet collection)


1965 reports on the code MUDE: Résolution de l'équation de la diffusion dans une géométrie à une dimension et calculs annexes[Solution to the Diffusion equation inlD-geometry and calculations] by Claude Bore, Yves Dandeu, Chantal Saint-Amand, report CEA-R 2923 (1965) and the code ALCI Spécification d'un code de diffusion multigroupe à deux dimensions [Specification for a 2D-multigroup diffusion code] by Jean-Paul Bayard et al report CEA-R 2747 (1965), These two codes were the angular stones of French reactor physics in the sixties. (The Marguet collection)


This poor quality A3 document is a rarity. It presents the manual chain of the codes of reactor physics at the French CEA in 1965. Upper wright shows the batches of punch cards of each reactor code. EDF could use them via an expensive computer link with the CISI Company, a division of the CEA. (The Marguet collection)

In 1971, P. Roussel of the Data Processing and Mathematical Studies (Traitement de l'Information et Etudes Mathématiques: TIEM) Department produced a multi-group 2D diffusion code with a triangular mesh for hexagonal fuel assemblies (13, 000 points), based upon the initial work of Feingold, and which led to the $U N G G$ CHERBOURG code. This was followed by the following for $U N G G$ studies: LISON, LANGEAC, DIAMANT in $2 D$, then BIBENDUM in $3 D$.


The Clamart site in May 1965, then known as the Laboratoires de recherches et stations d'essais de Fontenay [Fontenay research laboratories and test stations]. In the top right-hand corner near the water towers is the Reactor Physics Department building. (EDF)

There was also great interest in fast-neutron reactors. It must be remembered that the first reactor in the world to produce electrical energy was the EBR1 fast reactor located in Arco, Idaho (1951, using highly enriched uranium, cooled with a sodiumpotassium mixture, and producing 200 kWe for 1400 kWth . Jacques Montfort left for 1 year (1964-1965) to work on the Enrico Fermi rapid reactor in the United States, a metal uranium-based reactor with a power of 60 MWe which went critical in 1963; other engineers were assigned to Cadarache, wherein 1962 the CEA built RAPSODIE, which went critical in 1966 ( 20 MWth), and still others were associated with projects worldwide (Winfrith, ISPRA, GULF, etc.). One team specialised in $U N G G$ reactors (Bernard Noc, Matthieu Israël, Jean-Claude Chenal on thermal hydraulics, and so on). M. Vastel specialised in the digital processing of nuclear data. ${ }^{3}$ As attested by a publication in 1963 by Roger Pasquer, Estève Charrasse and Jacques Montfort, the Department of Nucleus Studies in Chatou mastered the analogue calculation of resonance parameters and inelastic cross sections. ${ }^{4}$

[^383]Although dependent on the Research and Development Centre in Chatou, the neutron physicists were detached to the Clamart site, near the computers which they filled up with impressive trays full of punch cards, for obvious practical handling reasons. Intensive use was made at the time for the $U N G G$ of the CHERBOURG code ( $2 D$ scattering, finite-difference 2-groups for triangular meshes) and the BARACA code for control rods. Ultimately, however it was the COREGRAF cell code at the CEA (Reuss et al) supplemented by the ALCI core diffusion code, which became the key codes for $U N G G$ facilities until these were abandoned in 1969.

In the middle of the $1960 \mathrm{~s}, E D F$ kept a very close eye on developments in fast reactors, but also in the water-cooled technology. The director of the sub-region of nuclear equipment, Jean-Pierre Roux, and his assistants, Claude Bienvenu and Boris Saïtcevski, managed to persuade Robert Boudrant, Director of Equipment, and Pierre Ailleret of the interest of ordering a reactor built using American technology, which required the purchase of enriched uranium fuel from the Americans, since this product was not available in France at the time, to the great displeasure of $C E A$, who saw it as a loss of national independence, while $E D F$ viewed it as an opportunity to vary its production modes (Floquet 1995, p. 28). There was even talk of a warfare between the two technologies: EDF (pro-water) and $C E A$ (pro-graphite) were forced to publish their report separately in the spring of 1967, since they could no longer harmonise their conclusion (Picard et al. 1985, p. 197). On April 3, 1967 EDF commissioned the CHOOZ A reactor (Westinghouse-type) 300 MWe , a protocol type like-water reactor built in an artificial cave beneath a mountain on the Belgian border, and operating with an unconventional fuel ( $15 \times 15$ rods with non-symmetrical cross control blades), for which calculation turned out to be a tour de force using APOLLO1. The reactor was built by the Equipment division, the engineering section of which was dubbed SEPTEN from 1968. At the same time, a heavy-water reactor was built in collaboration with the CEA at the Monts d'Arrée: Brennilis aka EL4 (EL for Eau Lourde/ heavy water) with an electrical power rating of 70 MWe , following on from the EL2 and EL3 piles in Saclay. However, the affair was driven chiefly by the CEA and the EDF teams comprised only 70 people (Larroque 1997, p. 279). The aim was to acquire experience with an intermediate power reactor producing high quantities of plutonium (because of its continual loading) using forced-march development tactics for fast reactors in the event of problems with uranium supply. The reactor worked extremely well until 1986 and is currently in the advanced stages of dismantling. At the start of the 1970s, some were thinking of also introducing boiling water reactors, which were studied at the Research and Development Division, but the oil crisis of 1973 and the good performance of CHOOZ A finally resulted in victory for the $P W R s$, which had a specific power six times greater than that of the French CEA-standard $U N G G$ and which posed fewer stability problems than the high-power BWRs.

## CODE NUCLEAIRE TRIDIMENSIONNEL JANE

D. FERNGOLD ot P. LARCHER

Electricite de France

## Notation.

Chaque milieu physique et chaque groupe d'Energie des neutrons est represente par un jeu de constante :
$D$ : coefficient de diffusion,
$\sigma^{a}$ : section efficace macroscopique d'absorption,
$\sigma^{R}$ : section efficace macroscopique de diffusion,
$\sigma^{f}$ : section efficace macroscopique de fission,
$\chi$ : elément du spectre de fission,
$X$ : integrale de l'elément du spectre de fission,
$\nu$ : nombre moyen de neutrons par fission.
Enfin, nous désignons par:
$G:$ le nombre de groupes.
Le groupe 1 étant le groupe rapide (haute énergie) et le groupe $G$ le groupe thermique (basse energio), $g$ designant un groupe quelconque.

$$
1 \leqslant g \leqslant G, \quad 1<G
$$

$\Phi$ : le flux de neutrons,
$\psi$ : la source de fission,
$\lambda$ : la valeur propre.

## Position du probleme.

On se propose de résoudre numériquement dans un parallélépipède rectangle les équations de la diffusion suivantes exprimbes dans un système de coordonnfes cartésiennes à 3 dimensions $(X, Y, Z)$

$$
\begin{gather*}
-D_{\theta} \nabla^{2} \Phi_{\theta}+\left(\sigma_{\theta}^{a}+\sigma_{\theta}^{R}\right) \Phi_{\theta}=\frac{\chi_{\theta} \psi}{\lambda}+\sigma_{\theta-1}^{R} \Phi_{\theta-1}  \tag{1}\\
\psi=\sum_{\theta=1}^{G}\left({ }_{\theta}\right)_{\theta} \Phi_{\theta} \tag{2}
\end{gather*}
$$

avec:

$$
1<g \leqslant G \leqslant 4, \quad \sigma_{0}^{R}=\sigma_{G}^{R} \equiv 0 .
$$

Presentation of the JANE code, the first-ever reactor physics code developed at EDF (Feingold and Larcher, circa 1963) (The Marguet collection)


Francis Vitton's thesis in experimental reactor physics (1967 on the CESAR (UNGG) tests) (The Marguet collection)

The teams of $E D F$ physicists were strengthened with the arrival in Equipment of J. Ryckelynck (1937-) following his PhD in reactor physics in 1965, and who became head of equipment at Fessenheim, and by the arrival in the Nuclear Studies Department of the $D E R$ of Jean-Paul Pasquet in 1962, who was no longer kept busy on code maintenance, and of Pierre François, Henri Mouney (1945-), Francis Hourtoulle and Gérard Gambier (1943-) in 1968, who had penned a prestigious state thesis on the progressive poisoning method as a perturbation method,
following his 3-year secondment to Cadarache, and he later became the Head of Department and EDF representative at EPRI.



#### Abstract

(Courtesy Gambier) Gérard Gambier's work on the theory of perturbation benefited from a quality edition in the collection of the internal notes of the DER. His work at Cadarache was considered so brilliant that it was suggested him to make it more profitable in the form of a state thesis (PhD), an extremely uncommon fact. Gérard Gambier assured the functions of Head of Reactors Physics Department during the detachment of Michel Perrin in the United States




This extremely praiseworthy popularizing book (1977) was written by Henri Mouney, former assistant-director of the Reactor Physics Department. (The Marguet collection)

Mention should also be made of Jean-Pierre Perrutel (1942-), ${ }^{5}$ who had an astonishing career (after entering the "École de Métiers" in Soissons in 1960, where he first learned to scramble up electricity pylons, he entered the $D E R$ in 1970 finally to become an research engineer in neutron physics, an exemplary path

[^384]which would be inconceivable today!). In 1972, the Nuclear Studies Department of DER/Clamart recovered the LEOPARD (1967) and FOG (1961) codes thanks to the ISPRA programs library. LEOPARD, a lattice code for $P W R$ developed by Westinghouse and used by its French licensed operator FRAMATOME, supposedly provided a better representation of burnable poisons than its CEA counterpart, EVEREST. FOG was a $l D$ four-group code providing an approach to the critical parameters (critical boron, radiotherapy, etc.). C. Ribas loaded them into the CDC 6600 calculator at the Clamart computer centre and compared them with the CEA's EVEREST/EVOE scheme from the CHOOZ A studies. The Reactor Physics Department then recruited Philippe Bioux (1948-), who was for a long time the head of the neutron physics group, and Michel Soldevila (1952-), who was one of the first people to study the neutron physics of $P W R s$ at DER and who specialized in plutonium recycling before joining the $C E A$. Furthermore, plutonium recycling in MOX marked a high point for the $D E R$, which had to convince the powerful and rather reticent Fuels Department of the feasibility of the affair. The studies by $D E R$, in collaboration with the CEA (Paul Reuss), resulted in zoning of the MOX assembly. At SEPTEN, development work was done particularly on the physics of $U N G G$ and then of $P W R$. We should mention above all Francis Vitton (1942-), who was recruited after his experimental thesis in the physics of $U N G G$ reactors following his DEA in reactor physics in 1965, and of Jean-Claude Lefebvre (1939-), the mind behind SEPTEN, and whom we have to thank for a great many of the physical model described in this work. Lefebvre helped design the JANUS code (1970) followed by JANUS 2 (1974) alongside G. Chevreau, a 2-energy group, 2D diffusion code for square meshes in $P W R s$ based on the American PDQ code (1957). JANUS 2, then 3, was an important code in the history of reactor physics at EDF. In 1978, the computer centre at Clamart ran it 700 times for fuel management for the three power plants in Fessenheim, Bugey and Tihange for a total of 30 h of calculations! These extremely modest figures by our modern standards nevertheless were of concern to the DER in 1979, who considered the code to be "all engrossing" and imagined itself swamped by the arrival of the several tens of new plants to come. I would also like to mention Serge Peytier, specialist in start-up

(Courtesy Jean-Pierre Perrutel)
study procedures, Antonino Vassallo (JANUS, SEBIBLIO et pre-versions of COCCINELLE) and Daniel Janvier, a great specialist in internal instrumentation. Regarding numerical development, Françoise Blanchon ${ }^{6}$ (1941-) with TIEM, joined the $D E R$ in 1964. She became the linchpin for the EDF neutronic codes, on which she worked for the rest of her career. After first working on the $U N G G$ codes, in 1977 she developed the POSEIDON 2D code for $P W R$, in order to replace the JANUS codes ( $2 D$ homogeneous for assemblies); the JASON/JONAS code (pin-by-pin, by J.M. Fabre of SEPTEN). COCCINELLE 3D, which she wrote beginning in 1982, was a direct successor to the functions of POSEIDON and handled the equation for diffusion for two energy groups and six delayed neutron groups (for kinetics) on a finite-difference basis. Françoise, with her very strong personality, was a major figure in the $P W R$ years at Clamart, as was the discreet but highly talented mathematician Jacques Planchard (1933-2009), whose multiple theoretical works on the diffusion equation and eigenvalue problems led him to write a reference textbook on the subject (Planchard 1995). In Reactor Physics, the main CEA codes used are RIFIFI ( $1 D, 2$ groups, analytic), ALCI ( $2 D$ multigroup, finite difference), and HETAÏRE for fast reactors.

[^385]
(Courtesy Blanchon)


The original report of the RIFIFI II code: Résolution sur IBM 7090 des équations de diffusion en théorie à deux groupes d'énergie et une variable d'espace [Solutions to the Diffusion equation with two energy groups and one space variable on IBM 7090] by Albert Amouyal, Marcel Bados, Thérèse Léna et François-Louis Mengin, note CEA-N 518 (1965). (The Marguet collection)

Jean Vergnes (1944-2004) specialized in the economic problems of the different plant designs (TIRELIRE code).

(EDF)
Jean Vergnes (1944-2004) spent practically his entire career at EDF R\&D, apart from a few years in recruitment. He was the first to focus on fuel-cycle economy and developed the TIRELIRE software for cycle management strategies, which is still used today. It was also he who promoted within EDF the concept of the AMSTER molten-salt reactor. He was the first neutron physicist at EDF to be named Senior Engineer, an honorary title very rarely bestowed. Despite his incapacitating (and finally lost) struggle with Parkinson's disease, he is remembered by all for his infectious enthusiasm about nuclear physics and his goodwill towards his colleagues

At the end of the 1970s, the Nuclear Studies Department, which has now become the Reactor Physics Department (PhR) in Clamart, devoted most of its efforts on the one hand to HTRs (Gambier, ALCYON code, although this sector would be abandoned following the setbacks with the 300 MWe American pilot reactor in Fort St Vrain, Colorado), and on the other to fast reactors (Pierre Cachera in Chatou from 1958, whose name would be given to the Cachera effect, that is ejection of corium via a central hole in $R N R$ fuel pellets in the event of core fusion). After a career in Equipment, he joined the SOFRATOME company created by Marcel Boiteux, director of $E D F$ from 1979 to 1987, to help with the exportation of FRAMATOME reactors abroad, and in fact comprising the Engineering division of $E D F$ ).

(EDF)
Pierre Charles Cachera (photograph circa 1962) gave his name to the physical effect of corium ejection though the central hole of the pellets in fast reactors, in case of severe accidents. This effect is believed to increase the safety as long as it mechanically extracts fissile material from the active core. Cachera actually wrote the article on Boiling Water Reactors (BWRs) in the French technical Encyclopaedia « Techniques de l'ingénieur », a subject of which he was one of rare specialists in France to have followed the failed French project in 1975 in Fessenheim

We should also cite some RNR specialists with SEPTEN (particularly Guy Vambenepe for fuel management). Diffusion codes were developed at the initiative of Gérard Gambier (who wanted to get free from the CEA) such as SUPERALCYON, ${ }^{7}$ CARDIFF (based on the English calculation kernel SNAP recovered by the $O C D E$ ). Jean-Michel Gomit (1954-), who was hired after his thesis on the release of fission products, became a recognised specialist in perturbation theory, before going on to take charge of the CRISTAL criticality code at IRSN.

In the 1970s and 1980s, the Physics of reactors department, aka PhR, was involved in the proliferation of studies in all possible fields: $U N G G$, gas and sodium $R N R, H T R$ using the English WIMS code, the thorium cycle, the AMSTER concept involving molten-salt reactors (Jean Vergnes), and then over-and under-moderated PWRs, not to mention hollow needles and other variants. Philippe Tétart (1957-) optimized the design of innovative reactors such as Under-Moderated Reactors and Convertible Spectral Shift Reactors. As a result of this specialization in "exotic" reactors, the interest of the Department ultimately shifted away from PWRs then under construction. However, this was not the case with SEPTEN, which developed diffusion codes for PWRs: LIBELLULE (ID diffusion, two groups) by Jacques

[^386]Fioroni ${ }^{8}$ (1951-), JANUS (2D diffusion, two groups) by Jean-Claude Lefebvre (1939-2011), Philippe Lebigot, and Roger Seban (1949-), with a state doctorate in Reactor Physics and then in Atomic Engineering in 1975, who went on to have a brilliant career in China. All of these codes were fed by a SEBIBLIO libraries generator using the CEA lattice code, APOLLO1.

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## THÈSE

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PRESENTÉE
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## A L'UNIVERSITÉ DE PARIS-SUD CENTRE D'ORSAY

pour obtenir<br>LE GRADE DE DOCTEUR ES-SCIENCES PHYSIQUES

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PAR
Gérard GAMBIER
La methode de l'empoisonnenent progressif come methode de perturbation pour la mesure des proprietes neutroniques d'un milieu multiplicateur
Soutenue le 27 Juin 1974 devant le Commission d'Examen
MM. J. HOROWITZ Prisident
J. BUSSAC
B. LAPONCHE
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The state thesis of Gérard Gambier (1974) (The Marguet collection)


The thesis of Michel Soldevila (1978) (The Marguet collection)

The $3 D$ COCCINELLE code was used in a project piloted by SEPTEN, in which only $D E R$ mathematicians were initially involved (mainly Françoise Blanchon, who wrote the first theoretical note in May 1982 with Jacques Planchard regarding the digital aspects).


Cachera's first patent $(E D F)$ of December 1972: the idea was to drill a central hole in the fuel pin to enhance corium flow. Simple perhaps, but someone had to think it up!

From mid-1987, the Reactor Physics Department changed tack completely. Jean-Pierre West, brilliant graduate of the "Ecole Centrale" and Head of Department at $P h R$, who had already been involved in the start-up of Superphénix, decided to set up a neutron diffusion code unit for $P W R s$ in a department which until then had been concerned solely with fast reactors and the design of advanced reactors, or $P W R$ studies.


## (Courtesy West)

Jean-Pierre West, after the École Centrale of Paris (1981), began his career in the Reactor Physics department ( PhR ) on the fast reactor fast SUPERPHENIX on the thorny problem of the calculation of the control rods worth. From 1987, he was named head of the neutronic group, a team of developers of PWRs codes. After a passage in the Division Nuclear Calculations, he returned as Department Head of PhR. After several executive positions in various divisions (SEPTEN, CNET, CNEN/SOFINEL), he was appointed Vice-president of the consortium UNISTAR created by EDF and Constellation Energy Group, asked to promote the construction of an EPR to Calvert Cliffs. The American energy context will become unfavourable to the project which did not succeed to this day. He was finally appointed Vice-Director of EDF/R\&D. We shall hold especially in this book its determining action to promote the 3D-diffusion COCCINELLE code inside the official calculation scheme of French PWRs. In a more personal way, he was the person who recruited me in 1987!

He recruited Danièle Verwaerde (1955-), an experienced engineer, from CEA/ $D A M$, who developed for COCCINELLE the conjugate gradient and pin-by-pin calculation methods, and myself, for whom neutron physics was by the time profoundly exotic! ${ }^{9}$ The new changes initially caused some upset at SEPTEN, which felt that it had been unjustly deprived of its code, but things settled down afterwards. Claude Garzenne (1956-) then developed the HOMERE transport/ diffusion equivalence, before being seconded to Cadarache on the important EPICURE experiment in plutonium recycling, while Michel Lam-Hime (1952-), one of the best neutron physicists at the Nuclear Calculations Division, created a chain out of the different neutron transport codes in the official chain, an industrialization process made necessary by the incredible complexity associated with the number of codes to be chained, and the increasing number of plants (up to 58). In mid-1986, an online monitoring code was created with recalibration, CAROLINE (Blanchon, Esclangon, Gomit, etc.), based on the same ideas as the American BEACON code. After several years of joint development at $M M N$ and $P h R$, this would prove to be a

[^389]technical success (calculation time less than real-time), though ultimately a failure, following abandonment of operational rollout for the French nuclear fleet, since the solution was considered too complex by the operator.


Thesis of Jean-Michel Gomit (1980) on contamination of the primary circuit of PWRs (The Marguet collection)


Thesis of Michel Lam-Hime (1981) on the particularly difficult problem of transport/diffusion homogenization (The Marguet collection)

In the 1990s, the most notable point was the development of nodal methods in COCCINELLE [Slimane Noceir (1964-)], the EFLUVE code for fluence on the reactor vessel, [Henri Schaeffer (1954-)] and the STRAPONTIN residual power code (myself). François-David Rosset (1957-), one of the best specialists on fuel loading, joined the Department.


The reference Textbook by Jacques Planchard (1995), with a preface by Robert Dautray (The Marguet collection)


Thesis of Jean-Louis Vaudescal (1993), future head of the PhR Department. (The Marguet collection)

In the numerical sphere, developments primarily concerned multi-group approaches (thesis of Jean-Louis Vaudescal (1964-), who became head of the PhR Department), as SEPTEN developed its expertise on accident methodologies
(Jean-François Gy ${ }^{10}$ (1967-), after graduating from Ecole Polytechnique in 1987, a major specialist in reactivity accidents) and on safety studies. Many EDF engineers taught on courses such as Atomic Engineering, and especially Applied Reactor Physics (of note is the extremely complete textbook by Nordine Kerkar (1967-) and Philippe Paulin (1957-) on the operation of $P W R$ cores). In the future, history may be marked by the new COCAGNE code ( $3 D$, multigroup, multi-solver), the fruit of an unfortunate collaboration with the $C E A$. While France's best neutron physics specialists have naturally gravitated together by definition at the $C E A, E D F$, being an operator, has built up recognised know-how in reactor physics that is very fortunately not limited strictly to the people cited.

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(EDF Sciences)
The book Exploitation des cæurs REP (Operation of PWR cores) by Nordine Kerkar and Philippe Paulin (2008), two of France's foremost specialists on this subject

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Louis Delherm, Nouveau traité d'électro-thérapie tome 1: généralités [New treatise on electrotherapy Part 1: general considerations], Masson. Paris, 1951, 1068 pages. This huge work in three parts is well known in the medical field. Part 2 and 3 are exclusively medical applications. Part 1 underlines the production of X-rays and their effects in matter. Part 1 has lots o illustrations on the radiotherapy and dosimetry of the time. The chapter on radiotherapy accidents is very instructive. A chapter on neutron absorption by living tissues is to be noted.
J.L. Delcroix, Introduction à la théorie des gaz ionisés [Introduction to the theory of inoized gases], Dunod. Paris, 1959, 170 pages. This book is a good beginning to plasma physics. First two chapters on collisions are very useful. The theory of free electron gas is preceded by a recall of the kinetic theory of gases.
Michelangelo De Maria, Fermi, un physicien dans la tourmente [Fermi, a physicist in the storm], Editions Belin - pour la science, ISBN 2-84245-049-3, 2002, 160 pages. An exceptional work
on the life of Enrico Fermi with numerous illustrations. This book depicts Fermi in the historical context of his time to show his genius, both as an experimentalist and a theorist.
Maurice Déribéré, Les applications pratiques des rayons infrarouges [Practical applications of infrared rays], Dunod. Paris, 1954, 3rd edition, 435 pages. This book which deals more with technical aspects than scientific ones presents numerous industrial applications.
J.A. DeSanto, Scalar wave theory: Green's function and applications, Springer. Berlin, ISBN 3-540-55263-4, 1992. En particulier le chapitre sur l'équation de Helmholtz.
Jean-Louis Destouches, Etat actuel de la théorie du neutron [Present state of neutron theory], Hermann. Paris, 1932. 68 pages. This book is as far as I know, the first neutron physics book in French, published the same year that Chadwick discovered the neutron!. He presents the knowledge of the time on the subject (Bothe and Becker experiment, Joliot-Curie experiments. . .) and analyses the proposed models (proton-electron dipole?). Very interesting.
La diffraction et diffusion des neutrons [Neutron diffraction and scattering], international colloque of Centre National de la Recherche Scientifique (CNRS), Grenoble September, 3-5 1963 CNRS Editions. Paris, 1964. 234 pages. This collection is dedicated to neutron crystallography and the analysis of magnetic structure. Phonon theory is also broached.
Bernard Diu, C. Guthmann, Danielle Lederer, Bernard Roulet, Physique statistique [Statistical physics], Hermann. Paris, ISBN 2-7056-6065-8, 2001, 1001 pages. The essential reference in kinetic theory of gases. The proof for Maxwell distribution and the properties used for thermalization are very useful to us. Several examples adapted for different physical phenomena. The author limits the use of quantum physics and abstract notations so that it easily accessible to beginners. Boltzmann is celebrated on the cover with a "strong" piercing look.
James E. Dodd, The ideas of particle physics: an introduction for scientists, Cambridge University Press. Cambridge, Royaume Uni, ISBN 0-521-25338-1, 1984, 202 pages. This book is a good starting point for particle physics with many illustrations.
Gustav Doetsch, Introduction à l'utilisation pratique de la transformation de Laplace [Introduction to the practical use of Lapalce transform], Gauthier-Villars. Paris, 1959, 198 pages. Table with lots of transforms for applications to differential equations.
Thomas James Dolan, Fusion research Volume I, II, III, Pergamon Press. Elmsford, USA, ISBN 0-08-025566-3, 0-08-025567-1, 0-08-028817-0, 1982, 855 pages + annexes. Volume I deals with theory, II with experiments and III with technological aspects.
Arnaud Doucet, Nando de Freitas, Neil Gordon, Editors, Sequential Monte-Carlo methods in practice, Springer. USA, ISBN 0-387-95146-6, 2001, 581 pages. It is a compilation of texts by several authors on the various applications of Monte Carlo.
H.R. Dowson, Spectral theory of linear operators, Academic Press, ISBN 0-12-220950-8, 1978, 422 pages. This mathematical textbook, easily accessible to the physicist (not always the case unfortunately) deals with linear operators.
Lawrence Dresner, Resonance absorption in nuclear reactors, International series of monograph in nuclear energy, Vol. 4, Pergamon press, USA, Library of Congress card number 60-14191, 1960, 132 pages. This volume is a classical text for resonance absorption. Crystal clear, it is THE reference for chapter 5.
James J. Duderstadt, Louis J. Hamilton, Nuclear reactor analysis, John Wiley, USA, ISBN 0-471-22363-8, 1976, 650 pages. Complete reference. I appreciate the clear notations. James Duderstadt is a great transport specialist.
James J. Duderstadt, William R. Martin, Transport Theory, John Wiley, USA, ISBN 0-471-04492X, 1979.
Stephen A. Dupree, Stanley K. Fraley, A Monte-Carlo primer: A practical approach to radiation transport, Kluwer Academic / Plenum Publishers, USA, ISBN 0-306-46748-8, 2002, 341 pages. Very useful to the Monte Carlo starter. Several programming source codes in Fortran are inserted. The most convivial reference on the subject.
Gaston Dupuy, Radium, Radioactivité, Energie nucléaire, collection Que sais-je, PUF, Paris, 1962, 126 pages. Written in 1941, the book dates quite a lot although updated in 1962.
M. Duquesne, R. Grégoire, M. Lefort, Travaux pratiques de physique nucléaire et de radiochimie [Practical work in nuclear physics and radiochemistry], Masson, Paris, 1960, 304 pages. Several experimental descriptions for radiation.
Emile Durand, Solutions numériques des équations algébriques, tome I: équations du type $F(x)=0$, racines d'un polynôme [Numerical solutions to algebraic equations Part 1: equations expressed as $F(x)=0$, roots of a polynomial], Masson, Paris, 1960, 327 pages. All is said in the title. An equation that cannot be dealt by techniques from this book would be a mathematical curiosity!
Emile Durand, Solutions numériques des équations algébriques, tome II : Systèmes de plusieurs é quations, valeurs propres des matrices [Numerical solutions to algebraic equations Part 2: equation systems, eigenvalues of matrices], Masson, Paris, 1961, 327 pages. One of the rare books in French to deal with eigenvalues.
P.A. Egelstaff (Editor), Thermal neutron scattering, Academic Press, London, United Kingdom, Library of Congress Card Number 65-14292, 1965, 523 pages. Analysis techniques for matter, neutron optics, crystallography.
P.A. Egelstaff, M.J. Poole, Experimental neutron thermlisation, Pergamon Press, Oxford, United Kingdom, Library of Congress Card Number 79-86201, 1969, 399 pages. Descriptions of several experiments on radiation detection.
Electron physics, Proceedings of the NBS Semicentennial Symposium on Electron Physics, held at the National Bureau of Standards on November 5-7, 1951, National Bureau of Standards Circular 527, USA, 1954, 416 pages. Especially for On the general theory of multiple scattering, particularly of charged particles by Ming Chen Wang and Eugene Guth, who developed the detailed $P_{n}$ solution with application to back-scattering. From my viewpoint, a paper that marked the history of transport theory.
M.M. El-Wakil, Nuclear power engineering, McGraw-Hill, USA, ISBN 07-019300-2, 1962, 556 pages. Deals with thermal hydraulic aspects and technologies. The first part deals with ractor physics. More relevant in thermal hydraulics than neutronics (the plots on page 67 on activity are not correct, a confusion with concentrations perhaps?).
P.M. Endt, M. Demeur, Nuclear reactions volume 1, North Holland, Amsterdam, 1959. A complete compilation of the reactions between neutron and matter, as well as scattering phenomena.
P.M. Endt, P.B. Smith, Nuclear reactions volume 2, North-Holland, Amsterdam, 1962.
A. Erdélyi (Editor), Higher transcendental functions, volume 1, McGraw-Hill, New-York, USA, Library of Congress Card Number 53-5555, 1953, 302 pages. Gamma function, Whittaker function, and so on.
A. Erdélyi (Editor), Tables of integral transforms, volume 1, McGraw-Hill, New-York, USA, Library of Congress Card Number 54-6214, 1954, 391 pages. Based on the famous shoebox of Harry Bateman, this book deals with the unusual Fourier and Laplace transforms.
Harold Etherington (Editor), Nuclear Engineering Handbook, McGraw-Hill, New-York, USA, 1957. 14 locally numbered chapters. Chapter 6: Reactor physics is within our framework.

Robley D. Evans, The Atomic Nucleus, McGraw-Hill, USA, ISBN 0-89874-414-8, 1955. This reference is almost exhaustive on the atomic nucleus, translated in French. The 1982 edition by Robert Krieger Publishing Company is easier to find.
P.V. Evans (Editor), Fast breeder reactors, proceedings of the London conference organized by the British Nuclear Energy Society, May 1966, Pergamon Press, London, United Kingdom, Library of Congress Card Number 67-15631, 1967, 951 pages. especially: F. Storrer, A. Khairallah, M. Cadilhac, J.M. Chaumont, P.P. Clauzon, et al : Physics, kinetics and shielding of fast breeder reactors -survey of recent work done in France, Fast Breeder Reactors, p 685-710.
Bernard Fernandez, De l'atome au noyau [From the atom to the nucleus], Ellipses, Paris, ISBN 2-7298-2784-6, 2006. 597 pages. This history book was written by a scientist and underlines the bibliography and the history of discoveries since radioactivity. A laudable work worth mentioning.

Jeol H. Ferziger, Paul F. Zweifel, The theory of neutron slowing-down in nuclear reactor, MIT press, Massachussets, USA, Library of Congress Card Number 66-13806, 1966, 307 pages. In my opinion, the best textbook on slowing-down. I recommend the notations.
Ulysse Filippi, Matière, rayonnement, énergie [Matter, radiation, energy], Dunod, Paris, 1965, 289 pages.
George S. Fishman, Monte Carlo, Springer USA, ISBN 0-387-94527-X, 1995, 698 pages. A very sober title for an excellent book on methods. It should be pointed out that there are algorithms descriptions for programming.
W.E. Fitzgibbon III, H.F. Walker (coéditeurs), Nonlinear diffusion, Pitman. San Francisco, USA, ISBN 0-273-01066-2, 1977, 232 pages. Especially the chapter Subcriticality for submultiplying steady-state neutron diffusion by P. Nelson for proving in diffusion theory that an undermultiplying medium means that the system is subcritical. (Honestly speaking, I always thought it was obvious!).
C.A.J. Fletcher, Computational Galerkin methods, Springer, New-York, USA, ISBN 0-387-12633-3, 1984, 309 pages. With applications to fluid mechanics.
Pierre-Henri Floquet, Histoire de la Centrale Nucléaire des Ardennes [History of the Nuclear Reactor of the Ardennes], Association pour l'Histoire de l'Electricité en France, Paris, ISBN 2-905-821-11-6, 1995, 193 pages. This book shows how EDF adopted water-moderated reactors: a technological adventure.
Anthony Foderaro, The elements of neutron interaction theory, MIT press, USA, ISBN 0-262-56160-3, 1971, re-edited 1979, 585 pages. The introduction is an amusing allusion to authors. This book is an impressive collection of theoretical models. The black cover is intimidating! The chapter on "collision kinematics" is a model for clear presentation that can be difficulty leveled. Foderaro presents collision within the quantum physics framework (Schrödinger's equation for which he analyses several solutions). He presents the BreitWigner model and the Doppler effect. In my view, one of the best textbooks on pure neutron physics.
Jacques Foos, Manuel de radioactivité à l'usage des utilisateurs Tome 1: l'atome et le noyau atomique [Radioactivity manual for users Part 1: the atom and atomic nucleus], Formascience, Orsay, ISBN 2-909336-02-6, 1993, 197 pages. Several exercises with review of lectures. For students.
Jacques Foos, Manuel de radioactivité à l'usage des utilisateurs Tome 2: les désintégrations radioactives, les interactions rayonnements/matière, les applications de la radioactivité [Radioactivity manual for users Part 2: radioactive decay, radiation/matter interaction, applications of radioactivity], Formascience, Orsay, ISBN 2-909336-04-2, 1994, 310 pages. Several exercises with review of lectures. For students.
G. Fournier, M. Guillot, Sur l'absorption exponentielle des rayons béta du Radium E [On the exponential absorption of beta rays of Radium E], Hermann, Paris, 1933, 37 pages. This study presents the modern approach for absorption of beams of electrons with several velocities by shields of aluminum and carbon of variable thickness. The continuous spectrum measured by Madgwick for the $\beta^{-}$emission by Radium E - the old name of bismuth 210 - is presented.
F.H. Fröhner, Evaluation and analysis of nuclear resonance data, NEA-OECD JEFF Report $18,2000,124$ pages. This book of high scientific value describes the theoretical models used for analyzing the resonances measured by experimentalists. He provides a summary of theoretical cross section models.
Fuel burn-up predictions in thermal reactors, proceedings of a panel held in Vienne, 10-14 April 1967, IAEA, STI/PUB/172, Vienne, Austria, 1968, 243 pages.
M. Salvy, L. Le Moigne, R. Marchal, Génie Atomique, cours fondamental, tome 1 [Nuclear engineering, fundamental lectures, part 1], INSTN/Presses Universitaires de France. Paris, Dépôt Légal $n^{\circ} 7806,1967$ (re-edited 1963), 440 pages. The INSTN has published an important collection of textbooks under the direction of Francis Perrin in the 1960's with sky-blue or green covers with most scientific knowledge of the time (neutron physics, materials, reactor physics, thermal conduction, reactor technology...). The second chapter Neutronics by Le

Moigne is a highly summarized form in 180 pages of knowledge that led to the construction of $U N G G$ reactors and which complements [Blaquière, 1962].
Aleksei Dmitrievich Galanin, Thermal reactor theory, Pergamon Press, USA, Library of Congress Card Number 58-12667, 1960, 3rd edition, 412 pages, translated by J.B.Sykes. A reference on mathematical considerations. The systematic use of neutron density rather than the flux is hard to understand at present. Units must be carefully dealt with (especially for the diffusion coefficient).
Denis-Jean Gambini, Robert Granier, Manuel pratique de radioprotection [Practical manual for radiation shielding], Tec\&Doc, Lavoisier, ISBN 2-7430-0161-5, 1997, 2 nd edition, 483 pages. Little theoretical considerations in this book aiming more at regulatory and practical aspects. The title is well suited for the book.
Noel Gastinel, Analyse numérique linéaire [Linear numerical analysis], Hermann, Paris, 1966, 364 pages. The last chapter deals with eigenvalue and associated eigenvectors calculations. It is unfortunate that there is no index.
Maurice Gauthron, Introduction au génie nucléaire [Introduction to nuclear engineering], INSTNCEA, ISBN 2-7272-0107-9, 1986, 365 pages. Very oriented towards practical cases with several examples. For the engineer more than the research scientist.
Les génies de la science (revue), Fermi, un physicien dans la tourmente, Les génies de la science, Pour la science, Belin, 2001, 98 pages. Each issue of "Génie de la science" is dedicated to a famous scientist. This one is a very interesting and fully illustrated issue on Fermi, mostly unknown to the general public.
Les génies de la science (revue), Einstein: le père du temps moderne, Les génies de la science, Pour la science, Belin, 2002, 96 pages. There is an impressive number of books dedicated to Einstein, but this book is a good review on the life and facts on Einstein.
Les génies de la science (revue), Maxwell: champ, particules, couleurs, Les génies de la science, Pour la science, Belin, 2005, 120 pages. Exciting!
Les génies de la science (revue), Planck : la révolution quantique, Les génies de la science, Pour la science, Belin, 2006, 120 pages.
Les génies de la science (revue), Niels Bohr: A l'aune de la physique atomique, Les génies de la science, Pour la science, Belin, 2008, 104 pages.
James E. Gentle, Random number generation and Monte-Carlo methods, Springer, USA, ISBN 0-387-21610-3, 2nd edition corrigée, 2005, 381 pages. The first two chapters on random number generators are very informative on the subject matter. Monte Carlo users often employ the random function of the coding language without knowing the theory behind. The problem of a biased distribution is also discussed.
Samuel Glasstone, Milton C. Edlund, The elements of Nuclear reactor theory, Mac Millan, USA, 1972, 416 pages. It is the re-edition of the 1952 version published at Van Nostrand.
Samuel Glasstone, Alexander Sesonske, Nuclear reactor engineering tome 1 et 2, Chapman-Hall, USA, ISBN 0-412-98521-7 et 0-412-98531-4, 1994, 841 pages in two parts, 4th edition. This reference is essential for reactor physics and was successfully edited several times. Glasstone published several work on the subject.
Bertrand Goldschmidt, Pionniers de l'atome [Atomic pioneers], Stock, Paris, 1987, 484 pages. Goldschmidt has been the only French who worked for the Manhattan Project on plutonium separation. He would become a very brilliant chemist at CEA and would propose the French solution. The photographs are somewhat deceiving (usual photographs, only those of the French coming to Canada are really interesting).
Herbert Goldstein, Fundamental aspects of reactor shielding, Addison-Wesley, Reading, USA, 1959, 416 pages. This reference book focuses on the theoretical considerations of radiation transport calculation, rather than medical ones - a good reference for chapter 3.
S.H. Gould, Variational methods for eigenvalue problems, Oxford University Press, London, United Kingdom, 1966, 275 pages. 2nd edition. Presents the Weinstein method and Rayleigh-Ritz method for estimating eigenvalues. The applications are destined for mechanics which is nevertheless an elliptic form equation similar to the diffusion equation.

Hartley Grandini Jr, Fundamentals of the finite element method, Macmillan, USA, ISBN 0-02-345480-6, 1986, 528 pages. Especially for Galerkin method. Very oriented for engineering purposes.
Walter Greiner, Ludwig Neise, Horst Stöcker, Thermodynamique et mécanique statistique [Thermodynamics and statistical mechanics], Springer, Heidelberg, Allemagne, ISBN 3-540-661662, 1999, 532 pages. Very didactic.
Pierre Grivet, Austin Blaquière, Le bruit de fond, Masson, Paris, France, 1958, 495 pages. The chapter on background noise and its mathematical representation is useful for understanding neutron noise.
S.K. Goduvov, V.S. Ryabenki, Theory of difference schemes, North-Holland, 1964, 289 pages.

Robert Guillien, Physique nucléaire appliquée [Applied nuclear physics], Eyrolles, 1963, 744 pages.
Louis A. Hageman, David M. Young, Applied iterative methods, Academic Press, New-York, USA, ISBN 0-12-313340-8, 1981, 386 pages. Conjugate gradient method, Chebychev acceleration, and so on.
D. Halliday, Introductory nuclear Physics, 2nd edition, was published by John Wiley, New-York, USA, Library of Congress Card Number 55-0365, 1955, french translation published by Dunod in 1957, translated by Robert Barjon.
Charlie Harper, Introduction to mathematical physics, Prentice Hall, New-Jersey, USA, ISBN 0-13-487538-9, 1976, 301 pages. This book corresponds to the requirements of engineers: no proofs which are hard to understand and numerous application examples. Very useful.
J.M. Harrer, Nuclear reactor control engineering, Van Nostrand - Argonne National Laboratory, Princeton, USA, 1963, 587 pages.
J.R. Harrison, Nuclear reactor shielding, Temple Press Limited, London, 1958, 68 pages. Contains the fundamentals of gamma and neutron radiation shielding, especially interesting analytical examples for neutron streaming in tubes, and rings.
B.G. Harvey, Introduction à la physique et la chimie nucléaires [Introduction to nuclear physics and chemistry], Dunod, Paris, 1964.
J.A. Harvey (Editor), Experimental neutron resonance spectroscopy, Academic Press, New-York, USA, Library of Congress Card Number 75-84151, 1970, 534 pages. Experimental measurements of cross sections up to 10 keV .
Alain Hébert, Applied reactor physics, Presses internationales polytechniques, ISBN 978-2-553-01436-9, 2009, 414 pages. After his Ph. D., Alain Hébert has worked at the CEA on transport problems and homogenization methods.
Heavy water lattices, specialists meeting held in Vienne, September 1959, IAEA, STI/PUB/17, Vienne, Autriche, 1960, 142 pages. Logically, Canadians from Chalk River present most papers at this meeting dedicated to heavy water reactors.
Werner Heisenberg, Nuclear physics, Philosophical Library, New-York, USA, 1953, 224 pages. It is more a popularizing work rather than academic one. There is a photograph of the old brewery with a lattice of chains containing uranium cubes in a reservoir of heavy water developed in Germany by Kaiser Wilhelm Institut (Wirtz, Bopp, Fischer, Jensen, Ritter) during the war for the Third Reich. A really interesting historical chapter. Several pictures are also presented.
B. Held, Physique atomique [Atomic physics], Masson, Paris, ISBN 2-225-82432-0, 1991, 228 pages. Especially Bohr atom.
Gabor T. Herman, Image reconstruction from projection : the fundamentals of computerized tomography, Academic Press, USA, ISBN 0-12-342050-4, 1980, 316 pages. On techniques of image deconvolution and the Radon transform.
Gerhard Herzberg, Atomic spectra and atomic structure, Dover, USA, ISBN 0-486-60115-3, 1991, 257 pages. It is the translation of a book published in German in 1937. There is a good description of quantum effects (Zeeman, Stark effects and a clear presentation of spin composition). A pioneer in molecular spectroscopy, this physicist was awarded the Nobel Prize in chemistry in 1971 for his work on internal geometry and the energy states of simple molecules, especially for free radicals.

David L. Hetrick, Dynamics of nuclear reactors, American Nuclear Society, La grange Park, USA, ISBN 0-89448-453-2, 1993, 542 pages, To my knowledge, the best textbook on reactor kinetics with [Keepin, 1965]. He develops several types of problems starting from the point-reactor. Essential to the neutron physicist.
Gerald J. Hine, Gordon L. Brownell (Editors), Radiation dosimetry, Academic Press, New-York, USA, Library of Congress Card Number 56-6605, 1956, 932 pages, the first three chapters are theoretical considerations.
A. Hitchcock, Nuclear reactor stability, Temple Press, London, United Kingdom, 1960, 61 pages, in the collection nuclear engineering monographs. Very oriented on the graphite-gas reactor of Calder-Hall. Off-topic: I hope that the author was not named Alfred!
Harry Hochstadt, Les fonctions de la physique mathématique, Masson. Paris, ISBN 2-225-373784, 1973, 290 pages. Completes [Abramowitz et Stegun, 1972] with useful proofs. Very useful: Bessel functions, the gamma function, orthogonal polynomials.
Banesh Hoffmann, with Helen Dukas, Albert Einstein, créateur er rebelle [Albert Einstein, creator and rebel], Seuil. Paris, 1975, 298 pages. Saying that Albert Einstein is the physicist of the 20th century is obvious. This book puts back his work in their historical context. Numerous photos.
K.H. Hoffmann, M. Schreiber, Editors, Computational statistical physics: from billiards to Monte Carlo, Springer, New-York, USA, ISBN 3-540-42160-2, 2002, 300 pages. It is a compilation of articles on the various subjects that as chaos on a billiards game, financial analysis or chaos in optical spectrum, with lots of Monte Carlo method: more for general knowledge in Monte Carlo than actual use for work.
James G. Holbrook, Laplace transforms for electronic engineers, Pergamon Press, Oxford, United Kingdom, Library of Congress Card Number 59-12607, 1969, 2nd edition, 347 pages. The applications are mostly in the fields of electricity or networking. There is a very complete table of transforms for real networks.
Homogenization methods in reactor physics, Proceedings of a specialists meeting on homogenization methods in reactor physics held in Lugano, Suisse, 13-15 November 1978. AIEA-TECDOC-231. Vienne, 1980, 670 pages. It is a compilation of articles on homogenization and equivalence methods for transport-diffusion calculations. Methods for reactors other than $P W R$ are also presented: BWR, etc.
Kenneth H. Huebner, The finite element method for engineers, John Wiley and sons, USA, ISBN 0-471-41950-8, 1975, 500 pages. The solution of the Helmholtz equation p253 is directly transposable to diffusion.
W. Hume-Rothery, Electrons, atomes, métaux et alliages [Electrons, atoms, metals and alloys], Dunod, Paris, 1959, 456 pages. One of the most peculiar physics book I ever read: it is a discussion between a young scientist and a metallurgist with much experience. Not academic but interesting.
Harry H. Hummel, David Okrent, Reactivity coefficient in large fast power reactors, American Nuclear Society, USA, Library Congress Card Number 73-119000, 1970, 386 pages. Very complete. This book is a must for specialists in accidentology.
Earl K. Hyde, Isadore Perlman, Glenn T. Seaborg, The nuclear properties of the heavy elements II: detailed radioactivity properties, Prentice Hall, USA, Library Congress Card Number 64-23184, 1964, 1107 pages les deux tomes. Every transuranium isotope is investigated. It completes the numerical databases by a description of measurements and physics comments.
M. Buernerd (Editeur), Instrumentation en physique nucléaire et en physique des particules [Instrumentation in nulcear physics and in particle physics], Notes from the Joliot-Curie school of nuclear physics at Maubuisson, September 26-30, 1988, Les editions de physique, Les Ulis, France, 1989, 553 pages. This book presents the state-of-the-art methods for detection systems. The text by J. Seguinot must be pointed out: Les compteurs Cherenkov, applications et limites pour l'identification des particules [Cerenkov counters, applications and limits for identifying particles].
R. Strumane, J. Nihoul, G. Gebers, S. Amelinckx (Editors), The interaction of radiation with solids, Proceedings of the international summer school on solid state physics held in Mol,

12-31 August 1963, North Holland, Amsterdam, 1964, 816 pages. This book presents the state-of-the-art methods for theoretical knowledge of damages created by the irradiation of solids. To be read especially for theoretical background, material science has changed much since.
Gérard Iooss, Daniel D. Joseph, Elementary stability and bifurcation theory (2nd edition), Springer-Verlag, Berlin, ISBN 3-540-97069-1, 1995, 324 pages.
Marius Iosifescu, Nikolaos Limnos, Gheorghe Oprişan, Modèles stochastiques, Hermes-Lavoisier, Paris, ISBN 978-2-7462-1611-2, 2007, 332 pages. Especially for Markov modeling.
S.L.S. Jacoby, J.S. Kowalik, J.T. Pizzo, Iterative methods for non linear problems, Prentice Hall. USA, ISBN 0-13-508119-X, 1972, 274 pages. Simplex, conjugate gradients, etc.
Eugene Jahnke, Fritz Emde, Tables of functions with formulae and curves, Dover, New-York, USA, 1945, 306 pages +76 pages of annexes. All the texts are in English or German. Useful for our applications of Bessel functions and the $W_{l}(\lambda)$ polynomials.
Raymond Jancel, Théo Kahan, Electrodynamique des plasmas fondée sur la mécanique statistique, tome 1 [Plasma electrodynamics based on statistical mechanics, Part 1], Dunod, Paris, 1963, 622 pages. Very clear and complete.
Peter A. Jansson, Deconvolution: with applications to spectroscopy, Academic Press, Orlando, USA, ISBN 0-12-380220-2, 1984, 342 pages. The inverse processing of measurements in spectroscopy requires advanced mathematical methods. This book is very accessible with numerous examples.
James Hopwood Jeans, Théorie dynamique des gaz [The dynamical theory of gases], Blanchard, Paris, 1925, 510 pages. This reference, although very old, is very detailed on the subject matter. To read for its historical viewpoint after [Diu et al, 2001].
Franck Jedrzejewski, Histoire universelle de la mesure [Universal history of measurements], Ellipses, France, ISBN 2-7298-1106-0, 2002, 416 pages. This work presents all the historical aspects of the units of measurements and their development over the centuries. The MKS system which became widespread in France after the Revolution is very well documented. Furthermore, other unusual units are also presented: for instance, we learn that the angle was an old unit for volume used in France in the Middle Ages to measure grains and that Germany proposed the benz for speed! The Dollar and the pcm for reactor physics are also correctly presented. Very interesting!
Abdul J. Jerri, Introduction to integral equations with applications, Wiley-Interscience, USA, ISBN 0-471-31734-9, 1999, 2nd edition, 433 pages. No example in neutronics is given in this book but the techniques for integral equations are very general. The first edition of this book was published at Marcel Dekker ( 254 pages). In the first version, the Green functions are discussed p95.
Irène Joliot-Curie, Les radioéléments naturels [The natural radioelements], Hermann, Paris, 1946, 187 pages. By the woman who discovered artificial radioactivity with her husband. The radioactive chains are also given, with old isotope names.
M. N. Jones, Spherical harmonics and tensors for classical field theory, Research studies press Itd, Letchworth, United Kingdom, ISBN 0 86380-028-9, 1985, 230 pages. Everything on spherical harmonics. Only one (minor) flaw: the font is very "typewriter"-like.
Marc Jouguet, Cours de physique tome IV: structure de la matière, Eyrolles, Paris, 1964, 262 pages. Especially for the complete description of the hydrogen atom and the chapters on nuclear physics.
Enrique Joven Alvarez, Dalton et la théorie atomique[Dalton and the atomic theory], Service clients, Grandes Idées de la Science, La Garenne Colombes, 2015, ISBN 978-2-8237-0244-6, 151 pages. A non-specialist book easy to read.
André Julg, Atomes et liaisons [Atoms and bondings], Armand Colin, Paris, 1970, 103 pages. At the frontier of chemistry and atomic theory, this book is very complete on chemical bondings, a subject which is quickly broached in other nuclear physics textbook. A particular introduction implies that obsolete theories must no longer be taught. I do not agree with the author on this point: from my point of view, understanding the mistakes (or approximations) of the past is essential to get to scientific truth and honing critical sense.

Georges Jurain, L'uranium [Uranium], Que sais-je collection, PUF, Paris, 1986, 126 pages. More directed towards geology. The ore refining to obtain the metal is well described.
Théo Kahan, Physique nucléaire et physique mésique [Nuclear physics and meson physics], Armand Colin, Paris, 1963, 222 pages. This small book may appear to be a popularizing work at first glance. It is not the case. Théo Kahan, a specialist of nuclear physics and quantum physics, has authored a very academic textbook with much information.
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Théo Kahan, G. Rideau et P. Roussopoulos, Méthodes variationnelles en théorie des collisions atomiques et en physique des réacteurs nucléaires [Variational methods for the atomic collision theory and nuclear reactor physics], Dunod, Paris, 1956.
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and attractive cover, this book contains a detailed list of the atomic tests of the time as well as a precise description of the accidents.
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Rosalynd Pflaum, Marie Curie et sa fille Irène: deux femmes, trois Nobel [Marie Curie and her daughter, Irène], Belfond, Paris, ISBN 2-7144-2885-1, 1992, 449 pages. Written by an American, thereby depicting the American fascination for Curie, this biography is very complete and tries to grasp the unbelievable fate of the Curie.
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Paul Reuss, Exercices de neutronique [Problem exercises in neutron physics], EDP Sciences, collection INSTN, Paris, ISBN 2-86883-706-9, 2004, 334 pages. A huge collection of exam problem with corrections and detailed comments.
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[^0]:    ${ }^{1}$ Glenn Theodore Seaborg (1912-1999) was an American chemist. After completing his PhD at Berkeley in 1937, he co-discovered the element plutonium and nine other elements in 1940 (with McMillan, Kennedy and Wahl), and identified more than 100 new radioactive isotopes. He was in charge of the plutonium chemistry department in the Manhattan Project during WWII that led to the creation of the second atomic bomb, which was dropped on Nagasaki on August the ninth, 1945. In 1946, he became head of the chemistry department at the Lawrence Radiation Laboratory. He was awarded the Nobel Prize in chemistry in 1951 and published more than 200 international papers, receiving countless scientific distinctions. He was listed in the Guinness Book of Records as the person with the longest entry in the Who's Who in America.
    ${ }^{2}$ In 1864, Meyer published his textbook: Die modernen Theorien der Chemie [Modern Theories of Chemistry], which contained a draft of his classification in order of atomic weight, but it was only in 1870, 1 year after Mendeleev, that he published a table highlighting the periodic relationship between weight and atomic properties. Rightly or wrongly, History has linked only the name of Mendeleev with the periodic table.

[^1]:    ${ }^{3}$ Antoine de Lavoisier (1743-1794) is an internationally recognized giant of French chemistry. He became a member of the French Academy of Science in 1768. In his study of combustion, Lavoisier demonstrated the roles of oxygen and nitrogen. He synthesized water and developed the well-known law of conservation of matter. His book Traité élémentaire de Chimie [Elements of Chemistry], written in 1789, is considered the first book of modern chemistry. His role as a tax collector under the French monarchy resulted in him being guillotined during the French Revolution after a peremptory judgment, during which the judge famously refused his request for a stay of execution that would enable him to finish a scientific project on which he was working, with the words "The Revolution has no need for scientists!". Below is a famous painting from David of Lavoisier and his wife in 1788.

[^2]:    Joseph Louis Proust. The French National Library
    ${ }^{5}$ Sir Frederick Soddy (1877-1956) was an English physicist who studied at Oxford. From 1900, he worked as Rutherford's assistant at the McGill Institute in Canada. Throughout this extremely fertile period, he investigated radioactive decay and established the concept of the isotope. He returned to England and taught at Oxford; he was awarded the Nobel Prize for chemistry in 1921.

[^3]:    ${ }^{6}$ Joseph John Thomson (1856-1940) is an English physicist who spent his entire scientific career in Cambridge. A graduate of Trinity College, he succeeded Lord Rayleigh in the chair of Experimental Physics at the famous Cavendish laboratory. He was awarded the Nobel Prize for physics in 1914 for his work on the electron and later on the electrical conductivity of gases. He was succeeded by his pupil, Rutherford, in 1919. His son, George Paget Thomson (1892-1975), also won the Nobel Prize for physics in 1937 for his co-discovery of electron diffraction, demonstrating wave-particle duality, and he thus joined the ranks of those illustrious parent-children couples each awarded a Nobel Prize (Niels and Aage Bohr, Marie and Irène Curie).

[^4]:    ${ }^{8}$ In the metric system, it is interesting to consult (Système métrique décimal 1930) for the history and (Jedrzejewski 2002) for the multitude of units. For conversions to the British Thermal Unit system, see (Wildi 1972). The 7 base units of the metric system are the meter (m), the kilogramme $(\mathrm{kg})$, the second ( s ), the ampere (A), the Kelvin (K), the candela (cd) and the mole (mol). All other units may be deduced from these. Subunits and supra-units are defined using the following prefixes: yocto $\left(y \equiv 10^{-24}\right)$, zepto $\left(z \equiv 10^{-21}\right)$, atto $\left(y \equiv 10^{-18}\right)$, femto ( $f \equiv 10^{-15}$ ), pico $\left(p \equiv 10^{-12}\right)$, nano ( $n \equiv 10^{-9}$ ), micro ( $\mu \equiv 10^{-6}$ ), milli ( $m \equiv 10^{-3}$ ), centi ( $c \equiv 10^{-2}$ ), deci ( $d \equiv 10^{-1}$ ), deca $\left(d a \equiv 10^{+1}\right)$, hecto $\left(h \equiv 10^{+e}\right)$, kilo $\left(k \equiv 10^{+3}\right)$, mega $\left(M \equiv 10^{+6}\right)$, giga $\left(G \equiv 10^{+9}\right)$, tera $\left(T \equiv 10^{+12}\right)$, peta $\left(P \equiv 10^{+15}\right)$, exa $\left(E \equiv 10^{+18}\right)$, zetta $\left(Z \equiv 10^{+21}\right)$ and yotta $\left(Y \equiv 10^{+24}\right)$. It should be said that the metric system (and cheese!) are seminal contribution of France to mankind.

[^5]:    ${ }^{9}$ The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles. The extremely interesting history of the mole is discussed in the doctoral thesis of Christiane Chabas-Buès: Histoire du concept de mole (1869-1969), à la croisée des disciplines physique and chimie, [History of the concept of the mole (1869-1969); at the threshold of physics and chemistry] published by ANRT, ISBN 978-2-7295-4586-4 (1999). The term mol was introduced in 1893 by Wilhelm Ostwald as an abbreviation of the German word molekul to designate the unit of molecule-gram, which was then translated as mole in English. The mole is the most recent SI base unit.
    ${ }^{10}$ Jean Baptiste Perrin (1870-1942) sat the French Agrégation examination in 1894 after studying at the "Ecole Normale Supérieure". In June 1897, he defended his doctoral thesis 'Cathode rays and Röntgen rays' just as French science was coming to the fore in this domain. He provided the

[^6]:    first experimental proof of the corpuscular nature of electrons and his work would later influence J.J. Thomson. In 1908, he determined Avogadro's number with great precision and was awarded the Nobel Prize in physics in 1926 for his work on the atom. He was very close to Paul Langevin and Marie Curie, with whom we share political affinities, and was one of the founders of the CNRS. His son, Francis Perrin, was a founder of the French CEA (Centre d'Etudes Atomiques), directing this organization from 1951 to 1970.

[^7]:    ${ }^{11}$ Friedrich Hasenöhrl (1874-1915) was an Austrian physicist who in 1905 produced the equation $E=3 m c^{2} / 4$ based on the work of Thomson, but which was corrected in 1914 by E. Cunningham. He was killed in the First World War. The Nazi regime later attempted to manipulate his work in order to put an Aryan gloss on Einstein's formula.

[^8]:    ${ }^{12}$ For more information on units in general and on the Universal System in particular, as well as related historical aspects, see (Jedrzejewski 2002).

[^9]:    ${ }^{13}$ Jean-Louis Destouches (1909-1980). After studying at the Faculty of Science in Paris, he obtained a degree in 1930 where he followed the courses given by Louis de Broglie. In 1933, he defended his doctoral thesis on super-quantification theories and then specialized in quantum mechanics. He entered the CNRS in 1936 as a research manager and worked on a general theory of particles. In 1938, he became a Doctor of Letters thanks to his thesis on "the general form of physics theories". In 1941, he completed a work on particles published by Gauthier-Villars, and 3 volumes on The fundamental principles of theoretical physics were published by Hermann in 1942. He taught both at the Faculty of Letters and Faculty of Science in Paris. In 1951, he expressed his reticence concerning the new orientations of L. de Broglie's theories. At the end of the 1970s, he proposed a solution to the Einstein-Podolsky-Rosen paradox concerning the functional theory of particles (according to an article by M. Bitbol: Jean-Louis Destouches, thé ories de la prévision et individualité, Philosophia Scientiae, 5 (1), pp. 1-30, 2001).

[^10]:    ${ }^{14}$ In the CGS system, $h=6.6260755 \times 10^{-27} \mathrm{erg} . \mathrm{s}$ where $1 \mathrm{erg}=10^{-7} \mathrm{~J}=1 \mathrm{~g} . \mathrm{cm}^{2} / \mathrm{s}^{2}$ (Berthelot 1956, p. 4).

[^11]:    ${ }^{15}$ Gustav Hertz was the nephew of Heinrich Hertz, author of authoritative studies on the photoelectric effect. At the end of the war, Gustav Hertz was captured, like many other German scientists, within the political sphere of the Soviet Union, where he was working on isotope

[^12]:    separation. At the end of his life, he was a professor in Leipzig in East Germany. James Franck, who was Jewish, was prescient enough to quit his position in Gottingen and emigrate to the United States immediately following the pogroms of 1933. He took part in the Manhattan project.

[^13]:    ${ }^{16}$ Although it has the merit of being simple, this image may nevertheless be misleading. Spin should be seen rather as an additional "spatial dimension" in the quantification phases (Julg 1970).
    ${ }^{17}$ Enrico Fermi: Considerazioni sulla quantizzazione dei sistemi che contengono degli elementi identici [Considerations on the quantization of systems containing identical elements], Nuovo Cimento 1 (1924), 145-152, FP 1:124-29.

[^14]:    ${ }^{18}$ Enrico Fermi:Sopra la teoria di Stern della constante assoluta dell'entropia di un gas perffeto monoatomico, Rend. Lincei 32 (2), 1923, 395-398, FP:1-114-17.
    ${ }^{19}$ Describing the position of the electron in its trajectory around the nucleus.

[^15]:    ${ }^{20}$ Hideki Yukawa: Interaction of elementary particles, Proceedings of the Physical and Mathematical Society of Japan No 17, pp. 48-57 (1935)

[^16]:    ${ }^{21}$ Maria Goeppert-Mayer (1906-1972) entered the University of Göttingen at the age of 17 years. David Hilbert, who lived next door to the Goeppert family, one day gave a talk on atomic physics which she attended. She was part of the circle of students under Max Born. In 1930, she completed her doctorate on the theoretical treatment of multiphoton processes. She married chemist Joe Mayer, whom she had met at Göttingen, and went with him to the USA. During the middle of an economic slump, she was unable to find a university post. In Baltimore, she welcomed Jewish physicists from Germany, who had begun to leave the country in 1933. Until 1941, she worked in an unpaid position in Columbia. In 1942 she was offered a position working for "Substitute Alloy Materials", whose secret aim was to develop processes for the enrichment of uranium 235 as part of the Manhattan Project. Teller invited her to take part in the "Opacity project" on the behavior of materials at very high temperatures within the context of the hydrogen bomb. She joined Fermi's team in Chicago, where she was given a post at the Argonne National Laboratory. She developed the calculations program for a breeder reactor on John Von Neumann's original ENIAC computer. Working with Teller on the origin of the elements, she discovered the magic numbers that led her to the theory for which she would be awarded the Nobel Prize in 1963. (Based on an article by Jonathan Tennebaum published in Fusion No. 51).

[^17]:    ${ }^{22}$ Regarding spin-orbit coupling in general, useful information is given in (Condon and Shortley 1959, p. 257).

[^18]:    ${ }^{23}$ For an accessible overview of HFB theories, see the article by M. Girod, J.P. Delaroche and J.F. Berger: Approches microscopiques en physique nucléaire [Microscopic approaches in nuclear physics], CHOCS journal No 4 from CEA/DAM (1992).

[^19]:    ${ }^{24}$ Claude Felix Abel Niepce, dubbed "Abel Niepce de Saint Victor" (1805-1870), was a French military man passionately interested in photography and chemistry and who carried out a great deal of research on the development of photographic plates and color fixation. He invented the so-called "heliochrome" process using chloride salts as color fixatives. However, photographs treated in this way did not preserve their colors, which turned grey on exposure to light. In 1841, he carried out experiments on cochineal to dye army clothing red. He then used various compounds to fix images on glass, steel and on paper using a process based on albumin, and which presented excellent resolution. From 1845, he attended the chemistry lessons given by Michel-Eugène Chevreul at the Natural History Museum in Paris, where Antoine then Edmond, and finally Henri Becquerel taught. His experiments led him to use uranium salts, after noting that the latter left an impression on photographic plates. He erroneously deduced from this a new action of light, which supposedly produced chemical "excitation" of uranium (1858 -"Quatrième mémoire. Sur une action de la lumière restée inconnue jusqu ici"' [Fourth dissertation. On a hitherto unknown action of light.], in Comptes rendus hebdomadaires des séances de l'Académie des sciences, vol. 47, pp. 1002-1006). Niepce published numerous dissertations and treatises on color binding, and was thus a major figure in the history of photography. Inevitable quarrels over who initially discovered radioactivity occurred between Niepce and Becquerel at the end of the twentieth century. After analyzing his studies, it seems fair to say that Niepce was the first observer, which is an incredible exploit when we consider the experimental means at his disposal at that time. However, the honor of finally explaining radioactivity clearly belongs to Henri Becquerel, who after numerous attempts, finally found the right path.

    On Niepce, see Paul Fournier, Josette Fournier: Hasard ou mémoire dans la découverte de la radioactivité ? [Chance or memory in the discovery of radioactivity?], Revue d'Histoire des Sciences, Année 1999 Volume 52, No. 1 pp. 51-80.

[^20]:    ${ }^{25}$ Henri Becquerel: Sur les radiations émises par phosphorescence [On radiation emitted by phosphorescence], Comptes rendus de l'Académie des Sciences, No. 46, p. 10, February 24, 1896.

[^21]:    ${ }^{26}$ Marie Sklodowska-Curie: Rayons émis par les composés de l'uranium and du thorium [Radiation emitted by uranium and thorium compounds], Comptes-rendus de l'Académie de Sciences, No. 126, p. 1101, April 12, 1898
    ${ }^{27}$ Pierre and Marie Curie: Sur une substance nouvelle radioactive contenue dans la pechblende [On a new radioactive substance present in pitchblende], Comptes-rendus de l'Académie de Sciences, No 127, p. 175, July 18, 1898
    ${ }^{28}$ Pierre and Marie Curie: Sur une nouvelle substance fortement radioactive contenue dans la pechblende [On a new highly radioactive substance present in pitchblende], Comptes-rendus de l'Académie de Sciences, No 127, p. 1215, December 26, 1898
    ${ }^{29}$ Marie Sklodowska-Curie: Sur le poids atomique du métal dans le chlorure de baryum radifère [On the atomic weight of the metal in radiferous barium chloride], Comptes-rendus de l'Académie de Sciences, No 129, p. 760, November 13, 1899

[^22]:    ${ }^{30}$ Lord Kelvin's calculations ignored the source of energy due to radioactivity, prompting Rutherford to reply tactfully towards the venerable elder scientist. A tabloid from the time made a playful reference to the subject of the scientific discussion in the title "Doomsday Postponed!"

[^23]:    ${ }^{31}$ W. Bothe and H. Becker: Künstliche Erregung von Kern $-\gamma$-Strahlen, Zeitschrift für Physik, n ${ }^{\circ} 66$, pp. 289-306 (1930)
    ${ }^{32}$ Irène Curie and Frédéric Joliot: Emission de protons de grande vitesse par les substances hydrogénées sous l'influence des rayons rtrès pénétrants [Emission of high-speed protons by hydrogenated substances under the influence of highly penetrating $\gamma$ rays], Comptes-rendus de l'Académie des Sciences, No 94, p. 273 (1932)
    ${ }^{33}$ James Chadwick: Possible existence of a neutron, Nature No 129, p. 312 (1932)
    ${ }^{34}$ Irène Curie and Frédéric Joliot: Un nouveau type de radioactivité [A new type of radioactivity], Comptes-rendus de l'Académie des Sciences, No 198, p. 254 (1934)

[^24]:    ${ }^{35}$ Salomon Rosenblum (1896-1960) Salomon Rosenblum begins his secondary education in Germany before leaving for Sweden where he begins a thesis on the ancient and modern oriental languages. A fortuitous meeting, in a café of Copenhagen with an assistant of Niels Bohr brings him to move into the sciences in Berlin by fascination for the new atomic science, then into Marie Curie Paris's laboratory in 1923. After a thesis (1928) on the attenuation of $\alpha$-beams through matter he resumes the study of the $\alpha$-ray spectrum of the Thorium C (the current bismuth 212), then Radium C (bismuth 214) by magnetic methods of his invention. The putting into service of the large electromagnet of the Academy of Science built supervised by Aimé Cotton and the use for the

[^25]:    first time in spectroscopy alpha of the method of focus in $180^{\circ}$, allowed him in 1929 to obtain an unequalled dividing power and to observe 4 different lines in the spectrum of the bismuth 214. Follows itself the discovery of the fine structure of the $\alpha$ spectrum, which lines are not unique as it was believed previously (the lines being very close possibly confused in a unique macro-line). He published his original works in the reference textbook (Rosenblum 1932). Of Jewish origin and naturalized French in 1929 thanks to the help of Marie Curie, Salomon Rosenblum spent 3 years of exile in the United States (1941-1944) during the German occupation of France. He eventually became friend with Albert Einstein. After the Liberation, he returned back in France as Director of a new laboratory CNRS(NATIONAL CENTER FOR SCIENTIFIC RESEARCH), at first to Bellevue where took place the first experiments on the neutrons post-war years in France, then in Orsay.

[^26]:    ${ }^{37}$ Enrico Fermi: Tentativo di una teoria dei raggi $\beta$ [Attempt at a Theory of $\beta$ Rays], Nuovo cimento, No 11, pp. 1-19 (1934)

[^27]:    ${ }^{38}$ Paul Ulrich Villard (1860-1934) was a French chemist who worked in the chemistry Department of the Ecole Normale in the "rue d'Ulm" in Paris. In 1900 he discovered within radium radiation a form of radiation unaffected by magnetic fields: $\gamma$ radiation. He entered the "Académie des Sciences" in 1908.

[^28]:    ${ }^{39}$ Yigal Ronen: The systematic behaviour of the spontaneous fission branching ratios of even-Z isotopes, Nuclear Science and Engineering, 160, 144-147 (2008). Ronen teaches at the Ben-Gurion University (Israel), where he specializes in the physics of minor actinides. Several of his reference books have been published by CRC.

[^29]:    ${ }^{40}$ P. De Marcillac, N. Coron, G. Dambler, J. Leblanc, J.P. Moalic: Experimental detection of $\alpha$-particles from the radioactive decay of natural bismuth, Nature, Vol. 422.

[^30]:    ${ }^{1}$ The index $s$ generally refers to data items relating to scattering.

[^31]:    ${ }^{2}$ L. Wolfenstein and J. Ashkin, Physical Review, 85, 947 (1952).

[^32]:    ${ }^{3}$ Care should be taken to record the energies (in the laboratory framework) before collision as $E$, and after collision as $E$, in accordance with the procedures for writing scattering integrals.

[^33]:    ${ }^{4}$ Sir Patrick Maynard Stuart Blackett (1897-1974) was an English physicist who completed his studies at Cambridge in 1921. He was extremely familiar with the experimental sciences in the dynamic setting of the Cavendish Laboratory, and thanks to his monk-like devotion to his work, which involved taking more than 20,000 photographs in his Wilson chamber, in 1925 he managed to identify only 8 collisions demonstrating the first transmutation of nitrogen-14 to oxygen-17 as a result of the capture of an $\alpha$ particle. Together with Guiseppe P. S. Occhialini, on February 7, 1933, he experimentally confirmed the existence of the positron, which had been discovered in cosmic rays by Carl D. Anderson in 1932. He was awarded the Nobel Prize for physics in 1948 for his work on cosmic rays, and he became President of the Royal Society in 1965.

[^34]:    ${ }^{5}$ Richard Babut: Modélisation des réactions ( $\alpha, n$ ) sur les noyaux légers pour déterminer la source inhérente d'un réacteur nucléaire [Modelling ( $\alpha, n$ ) reactions on light nuclei to determine the inherent source of a nuclear reactor], PhD thesis, Université Blaise Pascal (2002).

[^35]:    ${ }^{6}$ For an overview of ternary fission, a useful discussion is provided by N. Feather (Physics and Chemistry of Fission, 1969, p83).

[^36]:    ${ }^{7}$ The invention of the term barn for cross sections is ascribed to M.G. Holloway and C.P. Parker while they were working late into the night of December 1942 on the atomic bomb project in Los Alamos. "If a neutron is a tomato, then U238 has a cross-section as big as a barn!". Terms based on the names of key project leaders were thus narrowly avoided: the Oppenheimer, which was considered too long, or the Bethe, considered too. . . Greek!

[^37]:    ${ }^{8}$ Care should thus be taken to avoid calculating function $\sigma(E)$ with a change in the variable normally used in probability theory:

    $$
    \sigma(v) d v=\frac{\sigma_{0} v_{0}}{\sqrt{2 E / m}} d v=\frac{\sigma_{0} v_{0}}{\sqrt{2 E / m}} \frac{d E}{m v}=\frac{2 \sigma_{0} v_{0}}{E} d E=\sigma(E) d E
    $$

    since in this formula, the unit of the new functional $\sigma(E)$ is barns/(m.s ${ }^{-1}$ ), which is inconsistent with the unit of $I$. The exact calculation must thus incorporate $\sigma(E)$ expressed in barns.

[^38]:    ${ }^{9} \mathrm{pcm}=$ pour cent mille. This unit is used particularly to express the reactivity.

[^39]:    ${ }^{10}$ Otto Hahn, Fritz Strassman: Uber den nachweis und das verhalten der bei bestrahlung des urans mittels neutronentstehenden erdalkalimetalle [On the detection and characteristics of the alkaline earth metals formed by irradiation of uranium with neutrons], Die Naturwissenschaften, No 27, p. 11-15 (9 January 1939).
    ${ }^{11}$ Lise Meitner, Otto Frisch: Disintegration of Uranium by Neutrons: a New Type of Nuclear Reaction, Nature, No 143, p. 239-240 (11 February 1939).
    ${ }^{12}$ Hans Von Halban Junior, Frédéric Joliot, Lew Kowarski: Liberation of neutrons in the nuclear explosion of uranium, Nature No 143, p. 470-471, (8 March 1939).

[^40]:    ${ }^{13}$ R.J. Howerton, Nuclear Science and Engineering, 62, 438, 1977.

[^41]:    ${ }^{14}$ Reactor Physics Constants, ANL-5800, second edition, 1963.

[^42]:    ${ }^{15}$ J. Terrell, Fission Neutron Spectra and Nuclear Temperatures, Phys. Rev. 113, No 2, p. 527 (1959).

[^43]:    ${ }^{16}$ B. E. Watt, Phys.Rev. 87, p. 1037 (1952).

[^44]:    ${ }^{17}$ This relatively unorthodox term was used by staff managing the first French $U N G G$, stigmatizing the slow responses of the reactor, for example during the divergence stage.

[^45]:    ${ }^{18}$ A.C. Wahl (1985), Phys. Rev. C32, 184. For the record, Wahl is one of the co-discoverers of plutonium, along with Seaborg.
    ${ }^{19}$ In particular: Musgrove et al: Prediction of Unmeasured Fission Yields, Proc. Panel Fission Product nuclear Data, Bologna IAEA-169 2,163.

[^46]:    ${ }^{1}$ Concerning polarization, see (Filippi 1965, p. 101) and the work of the French physicist Etienne Malus (1808).

[^47]:    ${ }^{2}$ An illustration is provided by way of the x-ray applications used by the Department of Military Applications of CEA described in the journal CHOCS No 9 (December 1993). For the technical aspect of sensors, see Samueli et al. (1968).

[^48]:    ${ }^{3}$ Heinrich Rudolf Hertz (1857-1894) was a German physicist known for his work on electromagnetic radiation, including light. Born into a comfortably-off family in Hamburg, at the age of 6 years he entered the demanding School of Dr. Richard Lange. In 1872, he entered the prestigious Johanneum Gymnasium and obtained the Abitur in 1875. He then entered a construction engineering school but after reflection, signed up in for the University of Munich, where his mathematics teacher, Von Jolly, introduced him to the rigor of mathematics. He then studied under Von Helmholtz and de Kirchhoff in Berlin. Thanks to Von Helmholtz's training, he was awarded the gold medal of the Faculty of Philosophy for a study on electrical inertia. He defended his thesis on electrical induction: Über die induction in rotirenden kugeln (On the induction of rotating balls) in February 1880. He analyzed the problem of contact between two elastically and linearly deformable balls, a problem known as Hertzian contact stress. He then worked for 3 years as assistant to Von Helmholtz. He obtained a teaching position in Kiel for 2 years, after which he moved to Karlsruhe to become the assistant of future Nobel prizewinner, Karl Ferdinand Braun, and it was here that he carried out studies to verify that light is indeed a form of electromagnetic radiation. On November 13, 1886, he created the first wireless link using electromagnetic radiation produced by an oscillator and showed that these waves also travel at the speed of light. In 1887, he turned his attention to the photoelectric effect discovered empirically by Antoine Becquerel, but he is rightly considered to be the principal investigator in this field. These experiments, then those of his assistant, Wilhelm Hallwachs, are central to Einstein's theory of quanta of light and that of the photoelectric effect (initially known as the Hallwachs effekt). He died at a mere 37 years through septicemia that was doubtless caused by recurrent mastoiditis, before he had time to understand the significance of his experimental discoveries [Sources: article by R. Haidar in Photoniques No 56, pp. 21-23 (2011), "Heinrich Hertz, a Short Life" by Charles Susskind, San Francisco Press (1995)] (Public domain and the Marguet collection).

[^49]:    ${ }^{4}$ The term "photon" is derived from the Greek word for light. It was first used in 1926 by chemist Gilbert N. Lewis (1875-1946) in a theory. Although the theory was not confirmed, the term itself was immediately adopted by the scientific community.

[^50]:    ${ }^{5}$ William Henry Bragg was the father of William Laurence Bragg, cited earlier, with whom he shared the 1915 Nobel Prize in Physics "for their services in the analysis of crystal structure by means of X-rays."

[^51]:    ${ }^{6}$ Arthur Holly Compton (1892-1962) was an American physicist who obtained his doctorate in physics from the University of Princeton in 1916. He worked and taught at various universities, including Chicago (1923-1945), then Saint-Louis (1945-1961). His experimental and theoretical work on x-rays was considerable, earning him the 1927 Nobel Prize in Physics for discovery of the effect that bears his name.

[^52]:    ${ }^{7}$ There is an amusing anecdote about the fine structure constant. A journalist was interviewing Enrico Fermi one day and wished to take a photograph of the Master. In order to make the pose more credible, he asked Fermi to pretend to be writing an equation on the blackboard. Fermi played along graciously, but feeling uninspired, he wrote the formula for fine structure with the numerator and the nominator reversed and he mischievously mixed up the units $\alpha=\hbar^{2} / e c$ ! The picture incorporated this error in backstage, and we see Fermi smiling and drawing a vague geometric figure in which he inserts angle $\theta$ where he fancies, and clearly visible on the blackboard above his head sits the erroneous formula. That would have been fine, except that the United States Post Office later decided to create a stamp using this very photo in honor of Fermi after his death. The mistake was spotted too late and the stamp was issued. In a panic, the image on the stamp was corrected in order to limit the damage. As Rutherford famously quipped: "All science is either physics or stamp collecting".

[^53]:    ${ }^{8}$ This methodology was used in the GRACE code for the calculation of the attenuation of photons and the heating of the surrounding shielding of reactors, coded in Fortran on IBM 709 in 1959 by D.S. Duncan and A.B. Speir (Atomics International).

[^54]:    ${ }^{9}$ Y. Sakamoto, S.I. Tanaka, Interpolation of gamma-ray build-up factors for point isotropic source with respect to atomic number, Nuclear Science and Engineering, 100, p. 33-42 (1988).
    ${ }^{10}$ A. Assad, M. Chiron, J.C. Nimal, C. Diop, P. Ridoux: A new approximating formula for calculating gamma-ray buildup factors for multilayer shields, Nuclear Science and Engineering, 132, p. 203-216 (1999).

[^55]:    ${ }^{11}$ Thanks to the work of Andréas Schumm $(E D F / R \& D)$ on the MODERATO code.

[^56]:    ${ }^{12}$ On photoneutron cross sections, see: Rudy Lee Van Hemert: Threshold Phtoneutron Cross sections for light nuclei, PhD, University of California, 1968.

[^57]:    ${ }^{13}$ L.V. Spencer: Energy dissipation by fast electrons, National Bureau of Standards, USA, 1959.

[^58]:    ${ }^{14}$ O. Blunck, K. Westphal: "Zum energieverlust enrigiereicher elektronen in dünnen schichten" Zeitung Physik 130, p. 641 (1951).

[^59]:    ${ }^{15}$ Patrick Maynard Stuart Blackett (1897-1974) spent a great deal of time working on the characterization of cosmic rays and he was awarded the Nobel Prize for his work in 1948. After completing his studies at Cambridge in 1921, he conducted many experiments. He became President of the Royal Society in 1965, and was made a baron in 1965.

[^60]:    ${ }^{16}$ Russian physicist Pavel Cherenkov (1904-1990), who won the Nobel prize in Physics in 1958, together with I. Tamm and I. Franck for their physical explanation of the Cherenkov effect.

    Lucien Mallet (1885-1981) was one of the first radiologists in France. In particular, he developed radiotherapy in the field of cancer, going on to write a book on the subject: Les applications biologiques des corps radioactifs artificiels [Biological applications of artificial radioactive bodies]. In 1921, he worked with Dr. Robert Proust of the Hôpital Tenon in Paris on the development of a treatment for certain cancers involving radiotherapy. In 1926, he described the luminous radiation produced by a source of radium irradiating water which he attributed to the inexact nature of direct photons. He showed in 1928 that this radiation is continuous in energy. A Mallet prize was created in 1985 and is awarded by the "Fondation de France" for deserving work in the field of oncological radiotherapy.

[^61]:    ${ }^{17}$ Johannes (Hans) Wilhelm Geiger (1882-1945). German physicist. After his doctorate in 1906 in Erlangen, he left for England and studied terrestrial magnetism at Manchester University. It was here that he met Rutherford and became his assistant for experimental work. In 1912, he returned to Germany and worked at the National Institute of Science and Technology in Berlin on the detection of charged particles. It was in Kiel, from 1925 onwards, that together with his doctoral student, Walther Müller, he developed the famous proportional Geiger-Müller counter, whose clicking indicates the intensity of radiation being measured. In 1936, he was appointed director of the Technische Hochschule in Berlin. He was one of the key signatories of the Heisenberg-WienGeiger Memorandum of 1936, signed by many German scientists in protest against the poor image of theoretical physics in Nazi propaganda, which they attributed to the disdain of students for this subject. This memorandum ended such attacks and incited the regime to use physicists in the war effort rather than discouraging them. Indeed, Geiger, whether or not favorable to the regime, was a member of the German team that worked on developing the atomic bomb alongside Heisenberg.

[^62]:    ${ }^{19}$ Hans Geiger, Ernest Marsden: "On a Diffuse Reflection of the $\alpha$-Particles", Proceedings of the Royal Society, Vol. 82, pp. 495-500 (1909).

[^63]:    ${ }^{1}$ Emilio Gino Segrè (1905-1989) was an Italian physicist who started his career under Fermi, and who fled the fascist regime of Mussolini. He is the co-discoverer of the anti-proton. His significant works in theoretical particle physics earned him the Nobel Prize in 1959.
    ${ }^{2}$ Edoardo Amaldi (1908-1989) worked under Fermi after his engineering studies at Rome University. He defended his PhD thesis in 1929 on the Raman Effect of benzene. In 1937, he replaced Corbino as Professor of Experimental Physics at Rome University. Throughout the dark period of war, he tried to ensure that the Roman physics school remained. He worked on spectroscopy and detectors. A conference at La Sapienza University paid tribute to him in 2008.
    ${ }^{3}$ Franco Rasetti (1901-2001) followed the career of Fermi from Florence to Roma. He became the first assistant to Corbino, Professor of Experimental Physics. His specialization in experimental physics complemented Fermi's theoretical skills. In 1939, he left Italy for Quebec, where he became a world specialist on molecular spectroscopy. Although invited by his Italian friends Fermi and Segrè to join the Manhattan project in 1939, he vehemently refused on ethical grounds. His exceptional career is described in Franco Rasetti, physicien et naturaliste (Il a dit Non à la bombe) [Franco Rasetti, physicist and naturalist: the man who said "No" to the bomb] by D. Ouellet, Ed. Guérin (2000).
    ${ }^{4}$ Oscar d'Agostino (1901-1975) became a Doctor in Chemistry in 1926. After his work with Fermi, he joined the Italian National Scientific Research Center.

[^64]:    ${ }^{5}$ Bruno Pontecorvo (1913-1993) was one of Fermi’s youngest assistants. Like many Italian Jews, he fled fascism in his home country. Moving to the United States, already in 1942, while working for a petrol prospection company, he was seeking to develop a principle based on neutron emission. In 1948, he became a British citizen. In 1950, at the height of the "Cold War", he sensationally defected to the East with his family in unexpected and unexplained circumstances, despite having never worked on the bomb project. He was warmly welcomed In the USSR, where he specialized in high-energy physics until the end of his life.

[^65]:    ${ }^{6}$ The reader should note that not all references use the same definition of $\alpha$. For instance, (Weinberg and Wigner 1958) adopts the definition $\alpha_{w}=4 A /(A+1)^{2}=1-\alpha$, which makes transposition complicated. (Tait 1964, p12) prefers the notation $q$ to $\alpha_{w}$. In this book, $q$ is the slowingdown density.

[^66]:    ${ }^{7}$ In transport theory, angle $\psi$ is usually denoted by $\theta_{0}$ and its cosine by $\mu_{0}$. However, we differentiate here between this variable and the polar angle $\theta$ for the sake of clarity.

[^67]:    ${ }^{8}$ The specific slowing-down power is expressed by some authors as the moderation ratio, which risks being confused with the technological moderation ratio if the latter term is shortened.

[^68]:    ${ }^{9}$ For a theoretical background on Laplace transforms used in many physics problems, the reader is referred to (Doetsch 1959; Holbrook 1969; Kaplan 1962; Starkey 1954; Widder 1952).

[^69]:    ${ }^{10}$ S.A. Pozzi, I. Pazsit: Neutron slowing down in a detector with absorption, Nuclear Science and Engineering, 154, p367-373 (2006). After obtaining his PhD at the Roland Eötvös University in Budapest in 1975, Imre Pazsit, taught nuclear engineering at the University of Michigan, and then at the University of Chalmers in Sweden. He has written numerous articles dealing in particular with neutron noise, as well as a treatise on neutron fluctuations.

[^70]:    ${ }^{12}$ R.L. Murray, Nuclear Science and Engineering 128, p329-330 (1998)

[^71]:    ${ }^{13}$ The notation $R(E)$ is preferred here instead of the more common $F(E)$ (Glasstone and Edlund 1972; GA Vol. 1, 1967, p213), since it provides a mnemonic $(R(E)$ for slowing-down Reaction Rate).

[^72]:    ${ }^{15}$ E. Amaldi, E. Fermi, Physical Review. 50, p899 (1936).

[^73]:    ${ }^{16}$ In strict mathematical terms, the function $R_{s}(u)$ does not correspond to the same functional $R_{s}(E)$ where the variable $E=E_{0} e^{-u}$ has been changed. We have opted against overloading the text with new variables. The context in which the notations appear is thus essential for a correct understanding of quantities and their units.

[^74]:    ${ }^{17}$ G. Placzek, Phys. Rev., 69, p423 (1946).

[^75]:    ${ }^{18}$ John Von Neumann (1903-1957) was a Hungarian-born mathematician. As a child, he displayed prodigious mathematical skills. After his PhD in 1926 in Budapest, he left for Germany to work with the major physicists of the time. In 1930, he immigrated to the United States, where he worked at Princeton with Albert Einstein. He developed applied mathematics, then a thriving field with the advent of information technology, and he contributed significantly to numerical analysis and game theory, as well as economic analysis. He worked on the Manhattan Project, where his exposure to radiation is assumed to be the cause of his fatal bone cancer. (Public domain)

[^76]:    ${ }^{19}$ In practice, this is due to the fact that the flux results from a non-scattering flux added to a firstscattering flux, second-scattering flux, and so on to infinity in a non-absorbing medium, although the number of scattering events is obviously finite in a realistic medium.

[^77]:    ${ }^{20}$ Eugene T. Greuling studied at Duke University and obtained his PhD in 1942 from the University of Indiana (Theoretical Half-Lives of Forbidden beta-Transition), with Emil Konopinski as his doctoral advisor-himself a specialist of $\beta$ disintegration. As a specialist in nuclear physics, Greuling wrote his first article on the computation of permitted transitions for disintegrations using the tensor method as early as 1942 (Phys. Rev. 61-588 (1942). He was the doctoral advisor of Paul Frederick Zweifel (born 1929) in 1954 (Capture-Positron Branching Ratios), the wellknown author of several books on neutronics [among which (Case and Zweifel 1967)]. He contributed to the Manhattan Project at Los Alamos, then Oak Ridge. Greuling later taught physics at Duke University.
    ${ }^{21}$ Gerald Goertzel (1920-2002) obtained his PhD in theoretical physics from New York University. He was proficient in both numerical analysis and nuclear engineering. He was a member of the Manhattan Project, and later of the Nuclear Development Corporation of America. In addition, he developed medical instruments for Sage Instruments throughout part of his career. He then spent 28 years until his retirement at the research division of IBM devising algorithms for data compression. He designed the Goertzel algorithm, which helps identify the dominant cycles of a noise signal by computing the Fourier coefficients of multi-frequency sinusoidal signals inside the noise.

[^78]:    ${ }^{22}$ Martine Pujol (1941-1995) completed her Master's Degree in Reactor Physics in 1964-1965. She worked on her PhD at the CEA/Department of Pile Studies/Department of Mathematical Physics of Saclay, where she met Jean Bussac, Head of the Department, Oleg Tretiakoff, Michel Cadilhac, and Paul Reuss, then a young engineer. She later left the CEA to teach in Senegal, then at the University of Orleans. In 1971, she became a scientific journalist under the pen-name Martine Barrère for the scientific newspaper "La Recherche", where she worked in the "Science and Politics" section. She worked on several documentaries on nuclear power, the Soufrière volcano and AIDS. From 1979 to 1981, she presided over the Scientific Journalist Association. She left La Recherche in 1990 due to disagreements and worked as a freelance journalist for Le Monde amongst others. She taught scientific journalism at the University of Paris VII and contributed significantly to subjects dealing with Science or Consciousness. She died of cancer in 1995.

[^79]:    ${ }^{23}$ Jean Bussac (1929-). After his studies at the illustrious "Ecole Polytechnique" (promotion 1948), he was recruited in September 1951 to the «Commissariat à l'Energie Atomique » by Jacques Yvon au (CEA) where he participated in the developments of the mathematical theories applicable to nuclear reactors. In August, 1952, he participated in the International Seminar of physics of Les Houches in French Savoy (around thirty young scientists, some French people of whom future Nobel price Pierre-Gilles de Gennes). Appointed in 1962 head of the department of mathematical physics of the CEA, which he will lead at the top of the excellence in the field of the reactor physics, he went in 1972 to Oklo (Gabon) to study the natural reactor of uranium which produced fission there are 2 billion years. Having been the principal private secretary of the Highcommissioner of the CEA, he went to be the Director of Research for Nuclear Safety before retiring in 1984. He was also named Associated Professor at the University of Paris-XI and at the "Conservatoire National des Arts et Métiers". Writing en 1978 avec Paul Reuss the famous Treatise of Neutronics, republished several times, he also has written for the Encyclopedia Universalis with Jules Horowitz the article Nuclear reactors published in 1980 et he participated to the collective work L'aventure de l'Atome (the Adventure of Atom) published in 1992.

[^80]:    ${ }^{25}$ Michel Cadhilac, Martine Pujol: A simple model for the inelastic scattering of fast neutrons, Journal of Nuclear Energy, Vol. 21, pp58-63, 1967.
    ${ }^{26}$ Brigitte Rocca-Volmerange: After her PhD at the CEA in 1976, this French physicist turned to astrophysics. Today, she works at the Institut d'Astrophysique de Paris, where she specializes in the evolution model of galaxies. She teaches at the University of Paris XI in this field. Furthermore, she is also Vice-President of the association Femmes et sciences. [Women and Science]
    ${ }^{27}$ Brigitte Rocca-Volmerange: Approximation $Q_{n}$ du ralentissement dans les réacteurs nucléaires à neutrons rapides $\left[\mathrm{Q}_{\mathrm{n}}\right.$ approximation of slowing-down in fast-neutron nuclear reactors $], \mathrm{PhD}$ thesis at the University of Orsay, 1975.

[^81]:    ${ }^{1}$ P.L. Kapur, R.E. Peirls, Proceedings of the Royal Society (London), A166, 277 (1938).

[^82]:    ${ }^{2}$ Gregory Breit (1899-1981) was an American physicist of Russian origin. After working as Paul Ehrenfest's assistant at the University of Leide, he left for the United States, where he was a professor at a number of prestigious universities. His work on the Dirac equation led to a relativistic wave theory named after him. His work on resonance with Wigner led to the forms of Breit-Wigner cross sections. At the outbreak of war, Breit was the leader of the team of scientists that worked on the atomic bomb. Due to differences of opinion, he was replaced on the Manhattan Project by Robert Oppenheimer.

    Eugen Paul (Jenő Pálin Hungarian) Wigner (1902-1995) was a Hungarian physicist who immigrated to the United States. He joined the faculty of Princeton University and became a US citizen in 1937. The same year, he introduced the concept of total isospin tuples vector for nucleon

[^83]:    systems to improve understanding of nuclear reactions (Mathieu 1991, p. 234). In 1939, he was part of the group of five scientists (that included Albert Einstein) who warned President Roosevelt of the potential military use of atomic energy by Germany. During the Second World War, he contributed to the design of plutonium reactors and worked on the Manhattan Project. In 1963 he was awarded the Nobel Prize for Physics along with Jensen and Maria Goeppert-Mayer for the discovery of the symmetry principle. He belongs to the highly renowned Hungarian School of Physicists, along with Leo Szilard, Edward Teller and John von Neumann. Furthermore, he was one of the first to propose the use of water as a moderator and a coolant in reactors.
    ${ }^{3}$ For details on the Heisenberg uncertainty principle, see (De Broglie 1982).

[^84]:    ${ }^{4}$ G. Breit and E.P. Wigner: Capture of slow neutrons, Phys. Rev. 49, p. 519 (1936).
    ${ }^{5} g_{N}=2 I_{N}+1$ is the statistical weight of the target nucleus, and $g_{n}$ is that of the neutron $\left(g_{n}=2\right.$ $1 / 2+1=2$ ).

[^85]:    ${ }^{6}$ More precisely, the potential cross section is equal to $\sigma_{p o t}=4 \pi \lambda^{2} g \sin ^{2} \delta_{1}$, where $\delta_{1}=R / \lambda-\operatorname{Arctg}$ $(R / \lambda)$ is the neutron wavelength (not to be confused with the decay constant) and is the statistical weight of the compound nucleus.

[^86]:    ${ }^{7}$ L. Erradi: Etude des effets de température dans les réseaux caractéristiques des réacteurs nuclé aires de la filière à eau ordinaire['Study of the effects of temperature in representative lattices of light water reactors'], PhD, Orsay, 1982.
    ${ }^{8}$ On the distribution of resonances, Tran Quoc Thuong provides a very good reference: Analyse statistique des distributions des largeurs réduites partielles['Statistical analysis of the distributions of reduced partial widths'], Doctoral thesis, Université de Paris-VII (1973).

[^87]:    ${ }^{9}$ C.E. Porter, R.G. Thomas: Fluctuations of nuclear reaction widths, Phys. Rev. Vol. 104 n ${ }^{\circ} 2$ pp. 483-491 (October 1956).

[^88]:    ${ }^{10}$ A very good summary is provided in: Théorie de l'absorption résonnante des neutrons['Theory of resonant neutron absorption'], Technical report CEA-N-2679 (1991).

[^89]:    ${ }^{11}$ Igor Illich Bondarenko (1926-1964) was a Soviet physicist. After reading physics at the University of Moscow in 1950, he worked for the Institute of Physics and Energy in Obninsk. He studied the measurement of cross sections in the fast reactor framework. He finished his career as the ViceDirector of the Institute of Physics and Energy of the State Committee for the Control of Soviet Nuclear Energy. He was awarded the Lenin Prize in 1960. He was at the origin of the idea of the Fast Pulse Reactor which was built at Dubna. This reactor produced power peaks for a short time interval for experimental purposes. His work on cross sections was published in 1958 and was widely read in the west. It led to allowed comparison of calculations using the American evaluations. His cross sections were weighted in the resonance zone by self-shielding factors. Furthermore, his 26 -group energy structure was used at $E D F$ for the computation of power reactors.

[^90]:    ${ }^{12}$ This formalism is described in many references, but the work of Alain Santamarina is most suited for its clarity: Calcul de l'absorption résonnante des neutrons par les isotopes de l'Uranium et du Plutonium dans un réacteur nucléaire ['Calculation of the resonant absorption of neutrons by isotopes of uranium and plutonium in a nuclear reactor'], PhD., Orsay, 1973. Alain Santamarina (b. 1948) spent his entire career at the CEA after obtaining his Masters in reactor physics in 1971, followed by his PhD. A world-renowned specialist in nuclear data evaluations and neutron calculation schemes, he was at the head of the EOLE and MINERVE experimental reactors from 1984 to 1988. He subsequently became director of research at $C E A$. His recent works at Cadarache (France) led to the set-up of a new energy mesh structure with 281 groups for APOLLO2.

[^91]:    ${ }^{14}$ Historically, the notation was 0 for the resonant nucleus and 1 for the light moderator. We preferred to use uniform notations with $c$ for fuel (combustible), composed of $U$ for the heavy resonant nucleus (referring to Uranium, the main fuel component), and $m$ for mixed moderator and fuel, which is surrounded by an external moderator $M$.

[^92]:    ${ }^{15}$ For the sake of clarity, the models for the slowing-down operator are grouped in a later section so as to introduce the Livolant-Jeanpierre model first, along with the relevant notations.

[^93]:    ${ }^{16}$ Mireille Coste-Delclaux (b. 1956). After her studies in the mathematics section of the most famous "Ecole Normale Supérieure" in Fontenay (France), she passed the French "aggrégation" examination in mathematics, minoring in numerical analysis. She worked at the CISI Company, where she was involved in scientific programming languages. She later joined CEA/SERMA, specializing in problems dealing with nuclear data and self-shielding. Her PhD thesis at the CNAM: "Modélisation du phénomène d'autoprotection dans le code de transport multigroupe APOLLO2" ['Modelling of self-shielding using APOLLO2 multi-group transport code'] (2006) is the most complete reference on self-shielding in French, and it is a masterpiece of scientific work that would merit to be published in a textbook form. She has been a senior expert at CEA since 2005 and teaches neutronics at ENSTA, a French engineer school.

[^94]:    ${ }^{17}$ J. Chernick: The theory of uranium water lattices, Proceedings of the U.N. Conference on Peaceful Uses of Atomic Energy, Geneva, P603 (1955).

[^95]:    ${ }^{18}$ This concept will be described in more details in the chapter on the Boltzmann equation, and extended in the chapter on the heterogeneous reactor. The calculation is not detailed here. It is presented thoroughly in Wolfgang Rothenstein: Collision probabilities and resonance integrals for lattices, Nuclear Science and Engineering, 7, pp. 162-171 (1960).

[^96]:    ${ }^{19}$ George Irving Bell (1926-2000) was an American physicist. After obtaining his BSc in physics at Harvard University, he studied theoretical physics with Hans Bethe and obtained his PhD in 1951. He then worked for the theoretical physics division of Los Alamos in New Mexico. As a member of the T division, he worked on neutron transport and on the first thermonuclear bomb. In the 1960s, he worked on biology and immunology and indeed founded the theoretical biology and biophysics group in 1974. Similarly, in 1988, he was pivotal in the setting up of the Center for Human Genome Studies. In addition, he was very keen on mountaineering, and attempted the first ascent of the famous K2 (the attempt was thwarted by terrible weather conditions). However, in 1960, he took part in the first ascent of Mount Masherbrum.

[^97]:    ${ }^{20}$ The complete work of Mireille Coste-Delclaux on self-shielding is found in her PhD thesis: Modélisation du phénomène d'autoprotection dans le code de transport multigroupe APOLLO2 ['Modelling of self-shielding using the APOLLO2 multi-group transport code'], University of Orsay, (2006), edited by the CEA under reference number CEA-R-6114, 667 pages, which is the most complete French-language reference work on self-shielding.

[^98]:    ${ }^{21}$ M.N. Nicolaev, V.F. Khokhlov: A system of subgroup constants, Atomizdat, 1967
    ${ }^{22} \mathrm{~A}$. Hébert, M. Coste: Computing moment-based probability tables for self-shielding calculations in lattice codes, Nuclear Science and Engineering, 142, pp. 245-257 (2002)
    ${ }^{23}$ T. Ushio, T. Takeda: The characteristics and subgroup methods in square light water reactor cell calculations, Nuclear Science and Engineering, 143, pp. 61-80 (2003)
    ${ }^{24}$ O.K. Bouhelal and P. Ribon: Tables de probabilités non statistiques, description des effets du ralentissement ['Non-statistical tables: description of the effect of slowing'], Proc. Physor, Marseille, France, pIX-1 à IX-13, 1990. Pierre Ribon (b. 1932) graduated with an engineering degree from Arts et Métiers and ESE. After joining the CEA in 1956, in 1969 he defended his doctoral thesis,"L'étude de quelques propriétés des noyaux excités des noyaux composés, formés par l'interaction de neutrons lents avec le rhodium 103, le xénon, le gadolinium et le thorium 232" ['The study of certain properties of excited nuclei of composite nuclei formed through the interaction of slow neutrons with rhodium 103, xenon, gadolinium and thorium 232']. He is a renowned expert on nuclear data applied to reactor physics and although retired, he still maintains the CALENDF code package, the French equivalent of the American NJOY code.

[^99]:    ${ }^{25}$ Vladimirov (1979) is a good reference work on distribution theory.

[^100]:    ${ }^{26}$ Alain Aggery: Calculs de référence avec un maillage multigroupe fin sur des assemblages critiques par APOLLO2 ['Reference calculations with fine multi-group mesh for critical assemblies using APOLLO2'], PhD thesis at the University of Aix-Marseille (1999). A detailed description of the probability table method is presented in this thesis.

[^101]:    ${ }^{27}$ A. Khairallah, J. Recolin: Calcul de l'autoprotection résonnante dans les cellules complexes par la méthode des sous-groupes['Calculation of resonant self-shielding for complex cells using the subgroup method'], Proceedings of a seminar on numerical reactor calculations held in Vienna by the AIEA, 17-21 January 1972, pp. 305-317 (1972).
    ${ }^{28}$ Olivier Bouland: Amélioration du calcul de l'autoprotection des résonances résolues par un traitement quasi-exact du ralentissement des neutrons ['Improved calculation of self-shielding of resonances solved by quasi-exact approach of the slowing-down of neutrons'], PhD thesis, University of d'Orsay (1994).

[^102]:    ${ }^{1}$ Willis Eugene Lamb Jr (1913-2008) was an American physicist. He obtained his PhD on neutron scattering in 1938 at Berkeley under the supervision of Robert Oppenheimer, and published an original work in his own name on the effective temperature: Capture of neutrons by atoms in a crystal, Phys. Rev. 55, 190-197 (1939). He later taught at several faculties. He was awarded the Nobel Prize in 1955 for studies he performed in 1947 on the fine structure of the hydrogen atom concerning the doubling of hydrogen rays induced by virtual fluctuations of the electromagnetic field (second quantization). This effect is known as the Lamb shift.
    ${ }^{2}$ Peter Debye (1884-1966) was a Dutch chemist and physicist. He read electro-technics at Aachen under the supervision of Arnold Sommerfeld. In 1912, he derived the equations of the dipole moment in terms of temperature and developed a specific heat theory for very low temperatures by introducing the notion of phonons. In 1936, he was awarded the Nobel Prize in chemistry for "contributing to the study of the molecular structure through research on the dipolar moment and X-ray diffraction in gases." In 1938, he refused the insistent treaties of the Nazis to take German nationality and fled to the United States, where he worked at Cornell University and became head of the chemistry department. The Debye is the unit of the dipole moment of molecules

[^103]:    ${ }^{3}$ Woldemar Voigt (1850-1919) was a German physicist (Photo 6.2). At the University of Gottingen, his interests centered on crystallography and thermodynamics. In 1887, he published 'Über das Doppler'sche princip' (On the Principles of the Doppler Effect) in Göttinger Nachrichten (7), pp. 41-61 (1887), which was in fact one of the first theories involving non-varying speed of light, and thus prefigured the theory of relativity. In the same paper, he postulated the invariance of laws of physics in the translation frames. He suggested that the Michelson-Morley experiment in 1881 (showing that the Earth's motion had no effect on the speed of light) was due to Doppler effect within the absolute space-time frame, without nevertheless, although he did not challenge the principle of the ether-a medium with "magical" properties (harder than diamond, thinner than air!) that was postulated to explain the propagation of electromagnetic waves. Furthermore, he proposed a transformation of coordinates of a frame of reference that was also developed completely by Lorentz independently of Voigt. The name of Lorentz is still associated with this transformation. The work of Andreas Ernst and Jong-Ping Hsu on the history of sciences, First Proposal of the Universal Speed of Light by Voigt in 1887, Chinese Journal of Physics, vol. 39(3) pp. 211-230 (2001), shows the importance and Voigt's innovative work in its context, without diminishing the contributions of Lorentz or Einstein. For the record, it was Voigt who invented the word "tensor" in the mathematical sense in 1899.
    ${ }^{4}$ Beynon and Grant: Evaluation of the Doppler-Broadened Single-Level and Interference Functions, Nuclear Science and Engineering, 17, p. 545 (1963).

[^104]:    ${ }^{5}$ Dominique Grenèche: Physique des réacteurs à haute température, évaluation des sections efficaces résonnantes du Thorium 232, interprétation d'expériences critiques américaines [Physics of high-temperature reactors, evaluation of resonant cross sections of Thorium 232, interpretation of critical US experiments.], PhD thesis, University of Orsay (1973).

[^105]:    ${ }^{6}$ Historically, the quantity $\zeta$ was noted $i$, but the confusion with the complex number struck us as most unfortunate.

[^106]:    ${ }^{7}$ R. S. Keshavamurthy, R. Harish: Use of Padé approximations of the analytical evaluation of the $J$ $(\xi, \beta)$ function and its temperature derivative, Nuclear Science and Engineering, Vol. 115, pp. 81-88 (1993).

[^107]:    ${ }^{8}$ Arthur Ginsberg, Martin Becker: An improved series representation of Doppler-broadened resonance absorption, Nuclear Science and Engineering, Vol. 56, No. 1 pp. 106-107 (1975). The reader should pay careful attention to a small typing mistake in $A_{m} \equiv(-1)^{m} / \sqrt{1+m}$ and change the coefficient sign, since the equation should not be $A_{m} \equiv(-1)^{2} / \sqrt{1+m}$.

[^108]:    ${ }^{9}$ R. Bonalumi: Some Remarks about the Surface Resonance Absorption in Heterogeneous Reactors, Energia Nucleare, Vol. 12, No. 4, pp.189-204 (April 1965). In this work, Bonalumi develops the calculation of the effective area by taking into account the lattice effects. His approach uses the Dancoff effect and he proposes the use of correction coefficients for different moderators (water, heavy water, air).

[^109]:    ${ }^{10}$ Jean Mougey, Roberto Solanolla: Intégrale de résonance effective de l'uranium 238 [Effective resonance integral of Uranium-238], Note CEA-N 503 (1965).

[^110]:    ${ }^{11}$ Porter and Thomas, Physical Review No 104, 483 (1956).

[^111]:    ${ }^{12}$ T.P. Ribeiro de Campos, A.S. Martinez: Approximate calculation of the resonance integral for isolated resonances, Nuclear Engineering and Design, 102, 211-238 (1989).

[^112]:    ${ }^{13}$ A. Sanchez, A. Dos Santos: The intermediate resonance parameters for the multi-group formalism, Nuclear Engineering and Design, 387-400 (1999).

[^113]:    ${ }^{14}$ N.M. Steen, Nuclear Science and Engineering, 38, 244 (1969).

[^114]:    ${ }^{15}$ D. Neberejnev, C. Mounier, R. Sanchez: The influence of crystalline binding on resonance absorption and reaction rates, Nuclear Science and Engineering 131, pp. 222-229 (1999).
    ${ }^{16}$ H. Serizawa, K. Fukuda, T. Shiratori. T. Fujino, N. Sato and K. Yamada: Unusual variation of temperature factor of uranium dioxide at high temperature, Journal of Alloys and Compounds, Vol. 271-273, 1998, pp. 386-390.

[^115]:    ${ }^{17}$ This is the value in the American code MICBURN-E or deduced from the measurements made in the MINERVE reactor by H. Tellier.
    ${ }^{18}$ A. Meister, A. Santamarina: The effective temperature for Doppler broadening of neutron resonances in UO2, International Conference on the Physics of Nuclear Science and Technology, Long Island, USA, October 1998, pp. 233-239.
    ${ }^{19}$ G.M. Roe: The Absorption of Neutrons by Doppler Broadened Resonances, General Electric Company, Knolls Atomic Power Laboratory, KAPL-1241, New York, 1954.

[^116]:    ${ }^{20}$ A. Keane: Resonance absorption in a slab with a parabolic temperature distribution, Atomic Energy Research Establishment, AERE R/M 198, Harwell, UK, 1958.
    ${ }^{21}$ A. Reichel, A. Keane: Resonance absorption in a cylindrical fuel rod with radial temperature variation, Proceedings of the Royal Society, NSW 94, pp. 215-225, 1961.

[^117]:    ${ }^{22}$ G. Rowlands: Resonance absorption and non-uniform temperature distributions, Journal of Nuclear energy, parts A/B, 16, 235-236 (1962). After completing his PhD in theoretical physics on magnetism at the University of Leeds, George Rowlands (1932- ) joined Harwell in 1957, where he worked on fission first then on fusion. In 1966, he joined the University of Warwick where he taught non-linear physics problems and plasma physics until his retirement in 2000. He wrote a book on the latter subject: Nonlinear Waves, Solitons and Chaos, Cambridge University Press, 1990.

[^118]:    ${ }^{1}$ James Clerk Maxwell (1831-1879) was a Scottish physicist. He studied at the University of Edinburgh and took an early interest in the polarization of light. He completed his studies at Cambridge and taught as of 1860 at Aberdeen, then London, at King's College, where he developed a theory of electromagnetism for which he is world famous. His measurements of the speed of electromagnetic waves-which he noted was very close to that of light-led him to

[^119]:    postulate that light is a wave. The Maxwell equations are founding postulates of electromagnetism and relate electricity and magnetism, thereby constituting the first step towards unification of the various forces in physics. He died at 48 leaving behind him a significant body of work.
    ${ }^{2}$ Ludwig Eduard Boltzmann (1844-1906) was an Austrian physicist and a key figure in modern physics thanks to his work on statistical physics. After obtaining his PhD in 1866 on the kinetic theory of gases under the supervision of Jozef Stefan, he studied in Germany and then obtained the chair of physics at Graz. He established the famous equation of entropy in statistical thermodynamics $S=k \log \Omega$. A staunch defender of the atomic theory, he suffered from the misunderstanding of his theories. He suffered from depression and committed suicide in 1906. His name is associated with the Stefan-Boltzmann law for the power emitted by a surface as well as the Boltzmann integro-differential equation in the kinetic theory of gases, which may be applied to neutrons. His name is immortalized in the Boltzmann constant $k$, one of the rare constants governing the behavior of the Universe.

[^120]:    ${ }^{3}$ Mathematically, functional $n(E)$ is different from $n(v)$, but for the sake of clarity, the same terminology $n$ is used. Its units are defined according to the context in which it is used.

[^121]:    ${ }^{4}$ The density of thermal neutrons is of the order of $10^{7}$ to $10^{8}$ neutrons per $\mathrm{cm}^{3}$, which is negligible compared to the number of molecules per unit volume of the current moderator, even in gaseous form.

[^122]:    ${ }^{5}$ R.C. Tolman, Proc. Natl. Acad. Am. 11 (1925), 436.
    ${ }^{6}$ R.H. Fowler, E.A. Milne, Proc. Nat. Acad. Am. 22 (1925), 400.

[^123]:    ${ }^{7}$ V.V. Smelov, On the question of neutron thermalisation, Journal of Atomic Energy (USSR), 10, 1957.

[^124]:    ${ }^{8}$ Ernest Wilkins Jr (1923-2011) was an African-American mathematician who was extremely precocious (he attended the University of Chicago at the age of 13). In 1942, he obtained his PhD in mathematics at the age of 19 . He is in fact the 7th African-American to receive this distinguished title. At the same time, he obtained his Bachelor of Mechanical Engineering in 1942 at the University of New-York, which was followed by a Masters in the same field in 1960. He taught mathematics at the Tuskegee Institute from 1943 to 1944 . Wilkins was associated with the Manhattan Project from 1944 to 1946. He taught mathematics and carried out his research at the renowned Metallurgical Laboratory of the University of Chicago under the supervision of Enrico Fermi. From 1946 to 1950, Wilkins was in charge of mathematical studies for the American Optical Company; from 1950 to 1955, he was Senior Mathematician for the Nuclear Development Corporation of America. Furthermore, he was also responsible of the department of physics and mathematics (1958-1959), before becoming its director (1960-1965). Dr. Wilkins also worked for the department of theoretical physics at General Atomic from 1960 to 1970. In 1970, he was Distinguished Professor of Applied Mathematical Physics at Howard University. From 1974 to 1975, he served as President of ANS. In 1976, he was elected to the National Academy of Engineering of the USA. Besides his work in pure mathematics, he also worked in the 1940s to 1950s on the slowing-down and thermalization of neutrons, and then on photon transport and radiation protection.
    ${ }^{9}$ Eugène Paul Wigner, J. Ernest Wilkins Jr: Effect of the temperature of the moderator on the speed distribution of neutrons with numerical calculations for H as a moderator, AECD 2275 (1944).

[^125]:    ${ }^{10}$ Jules Horowitz (1921-1995) is considered by many as the father of reactor physics in France. A brilliant physicist, he joined the $C E A$ in 1946 after graduating from Ecole Polytechnique, where his studies were interrupted by the war. He joined CEA at the same time as Michel Trocheris, Claude Bloch and Anatole Abragam, with the group being known collectively as the "Three Musketeers" (Lefebvre 2002, p33). He laid down the founding elements of reactor physics by calculating the Zoé pile on the advice of Lew Kowarski. During his work on experimental reactors as director of the atomic piles, his requirements led to the introduction of the first scientific computers in France at the department of mathematical physics, where they were developed by Albert Amouyal (Lefebvre 2002, p116). His scientific work has been re-edited in the collection of important actors at the CEA. The new materials test reactor presently being built at Cadarache bears his name.
    ${ }^{11}$ Oleg Tretiakoff, a former student at the Ecole Polytechnique (1950-1952), was an engineer in the Armaments Corps at the French Defense Ministry. He remained at the CEA throughout his whole career (1955-1981), retiring as Chief Weapons Engineer. In 1975, with his wife he invented a piezo-electric system that allows the decoding of text printed in Braille for the blind. He applied for a patent in 1977. Nowadays, he lives in Florida where he heads a company working on these concepts.
    ${ }^{12}$ J. Horowitz, O. Tretiakoff: Effective cross sections for thermal reactors, European American Nuclear Data Committee, EANDC (E) 14, 1960, referred to in the work of Jules Horowitz. See also Francis Vitton: Mesures d'indices de spectre à César [Measurement of the Cesar spectrum indices]. His PhD thesis at the University of Orsay (1967) describes the complete model.

[^126]:    ${ }^{13}$ Michel Cadilhac: Méthodes théoriques pour l'étude de la thermalisation des neutrons dans les milieux infinis et homogènes [Theoretical methods for the study of neutron thermalization in infinite and homogeneous absorbing media], PhD thesis at the Faculty of Science of Paris (1964) and CEA technical report referenced as CEA R 2368. Michel Cadilhac (1934-) studied at the Ecole Normale Supérieure in Saint-Cloud before passing his aggrégation (competitive examination to become a lecturer). He joined the $C E A$, where he developed several theoretical notions related to thermalization (diffusion coefficient, spectrum, etc.). His thesis on the subject was presided by Jacques Yvon, assisted by Jules Horowitz and Austin Blaquière as examiners. It contained highly innovative ideas for the time and improved the Wigner-Wilkins model, making it one of the most important theses in French neutron physics. His work has been translated into English (Theoretical methods for the study of neutron thermalization in infinite and homogeneous absorbing media, Euratom translation EURAEC-1203, 1963). As a professor at the University of Marseille, he focused on the diffraction of electromagnetic waves in crystals.

[^127]:    (The Marguet collection)
    ${ }^{14}$ M. Cadilhac, J. Horowitz, J.L. Soulé: Some mathematical and physical remarks on neutron thermalization in infinite homogeneous systems, Conference on neutron thermalization, Brookhaven (April 1962).

[^128]:    ${ }^{15}$ Jean-Pierre de Brion: Application du modèle secondaire à la thermalisation en milieu hété rogène [Application of the secondary model to thermalization in heterogeneous media], PhD thesis at the University of Paris, 1966.

    Jean-Pierre de Brion (1936-1998). After his studies at Polytechnique (entry year 1957), he completed his military service in Algeria before joining the CEA around 1961-1962. In November 1964, he authored technical report SPM No 306: "Calcul de la densité neutronique dans une cellule hétérogène [Calculation of neutron density in a heterogeneous cell]". He defended his thesis on March 2, 1966 with a jury composed of Jules Horowitz, and Austin Blaquière and Oleg Tretiakoff as examiners and Michel Livolant as an invited member. In 1970, he married Monique

[^129]:    ${ }^{16}$ REMARK—For heavy nuclides, $\xi \approx 2 / A$.

[^130]:    ${ }^{17}$ Coveyou, Bate and Osborn, in Reactor Physics Constants ANL-5800, p89, obtained from the Monte Carlo calculations for moderators of different masses.

[^131]:    ${ }^{18}$ Carl H. Westcott (1912-1977) graduated from Cambridge in 1933 and started his career at the Cavendish Laboratory. He worked from 1937 to 1940 at the University of Aberdeen, then specialized in radar technology during the war. He co-authored a book on the subject in 1948. In 1944, he immigrated to Canada and became a professor at the McGill Institute at Montreal in 1949. In 1954, he joined the Chalk River center where he specialized in the processing of cross sections. Other than the formalism that bears his name, he was at the origin of the idea that a linear accelerator can simultaneously accelerate positive and negative ions, thereby significantly increasing the potential value of such machines.

[^132]:    ${ }^{19}$ C. Wagemans, P. Schillebeeckx, A.J. Deruytter and R. Barthélémy: The Subthermal neutron induced fission cross sections of the common fissile isotopes and their impact on the Westcott $g$-factor, Nuclear data for science and technology (1988 Mito), 91-95 (1988).

[^133]:    ${ }^{20} \mathrm{P}$. Cogné: Etude des caractéristiques nucléaires de l'empilement critique MARIUS [Study of the nuclear characteristics of the Marius critical pile], technical report CEA/SPM No 567, August 1959. For the general properties of graphite, see (Reynolds 1968).

[^134]:    ${ }^{21}$ I.M. Cohen, M. Arrondo, M.A. Arribère, M.C. Fornaciari Iljadica: A method for fast determination of the $\alpha$ parameter in nuclear reactors, Nuclear Science and Engineering, 154, p110-117 (2006).

[^135]:    ${ }^{22}$ C.H. Westcott: Effective cross section values for well-moderated thermal reactor spectra (3rd edition, corrected), CCRP-960, November 1960.

[^136]:    ${ }^{1}$ Ludwig Eduard Boltzmann (1844-1906) was an Austrian physicist born in Vienna. He is the father of Statistical Physics and stoutly defended the atomic theory of matter. After a PhD in 1866 on the kinetic theory of gases under the supervision of Josef Stefan (another brilliant scientist in the field of thermodynamics), he became the Chair of theoretical physics, then Mathematics, in Vienna, before moving to become the Chair of experimental physics in Graz-a town that had a special place in his heart. He approached thermodynamics from a revolutionary point of view by establishing the entropy law $S=k \log \omega$, which was named after him. Having an intense personality, the turbulent discussions brought about by his work submerged him in various bouts of depression. Well ahead of his time but having a tortured personality, Boltzmann took his life in 1906 in Duino, near Trieste, maybe owing to the indifference or lack of understanding that had followed his theories. History, however, will prove him right with the amazing progress of atomic science in the first 40 years of the twentieth century. And while he had never even fathomed the existence of the neutron, the neutronics field owes him much through his contribution of the very

[^137]:    important equation governing the behavior of neutrons. The scientific community, recognising his substantial contribution, gave his name to the fundamental constant, $k$, which occurs in the entropy law.
    ${ }^{2}$ Kenneth M. Case (1923-2006), after his studies at Harvard, contributed to the Manhattan project, before defending his PhD in 1948. Professor of chemistry from 1952 to 1967 at the University of Michigan, he was then appointed Professor of Applied Physics at the Rockefeller University of New York in 1967 where he stayed until the end of his career. Member of the National Academy of Sciences in 1975, Case was an expert in non-linear equations and contributed significantly to the neutronics field as well as in fluid mechanics (Burger equations) or in quantum mechanics (Benjamin-Ono equations). On a more anecdotal note, his name was associated in the 70's with the Jason project-a group of scientists working for the government on top-secret projects (UFOs and so on), something which still fuels the imagination of the general American public.

[^138]:    ${ }^{4}$ J. Kenneth Shultis: After a Ph.D. at the University of Michigan in 1968, he worked in several fields linked to neutronics, in particular, Monte-Carlo methods in transport and radioprotectionfields in which he published numerous articles. He now teaches nuclear engineering at Kansas State University and is the author of several reference books.

[^139]:    ${ }^{5}$ Regarding the approximations made for the derivation of the Boltzmann equation, the author highly recommends (Decoster et al. 1998), in particular the section on the limit of BoltzmannGrad. The latter shows that the collision term of the equation is justified for a number $N$ of interacting particles that tends to infinity. In the case of the hard sphere model of gases, where the radius of a particle is given by $a$, if the area $N a^{2}$ is constant, this means that $a$ tends to zero-from which stems the consequences on the way of measuring space (and time) with respect to a characteristic spatial dimension (and time).

[^140]:    ${ }^{6}$ For the concept of solid angles, the author recommends (Baur 1985, p18), which examines the calculation in detail.

[^141]:    ${ }^{7}$ For one energy group, $\chi=1$, but it has been left here to remember to take into account the fission spectrum in case of generalizing to a multi-group problem.

[^142]:    ${ }^{8}$ D.C. Sahni: Some new results pertaining to criticality and time eigenvalue of one speed neutron transport equation, Progress in nuclear energy Vol. 30, n ${ }^{\circ} 3$, 305-320 (1996).

[^143]:    ${ }^{9}$ The $\gamma$ notation is sometimes used but Dahl and Sjöstrand prefer using the $c$ notation in Nuclear Science and Engineering 69, 114 (1979). The $c$ notation is becoming more and more widespread, $c$ being the number of secondary neutrons.

[^144]:    ${ }^{10}$ The author preferred using the notation $\ell$ as the integration variable along the direction $\vec{\Omega}$ rather than the notation $R$, which is overused in numerous reference textbooks.

[^145]:    ${ }^{11}$ The optical path is often denoted by $\tau$ in numerous texts. The $\overline{\Sigma_{a} \ell}$ notation was preferred here since the physical meaning is retained. Stacey (2001) uses $\alpha\left(r, r^{\prime}\right)$.

[^146]:    ${ }^{12}$ For the mathematical aspects of perturbation theory, refer to (Bellman 1964; Cole 1968; Nayfeh 1973).
    ${ }^{13}$ See also E. Greespan: Perturbation theory and importance functions in integral transport formulations, Nuclear science and Engineering, 61, pp170-180, 1976.

[^147]:    ${ }^{14}$ G.B. Bruna, J. Planchard: Flux neutroniques dans un réacteur légèrement sous-critique en pré sence de sources [Neutron flux in a slightly subcritical reactor in the presence of sources], Research and Studies department bulletin, series C, No. 4, p55-67 (1990).

[^148]:    ${ }^{15} \mathrm{~J}$. Planchard: Calcul des flux neutroniques dans un réacteur au voisinage de la criticité and en présence de source [Calculation of the neutron fluxes in a reactor in the neighbourhood of criticality in the presence of sources], Research and Studies department bulletin, serie C, $\mathrm{N}^{\circ} 2$, p11-16 (1989).

[^149]:    ${ }^{16}$ Tabulations of exponential functions can be found in numerous mathematical textbooks, but also in some radioprotection textbooks such as (Goldstein 1959, p353).

[^150]:    ${ }^{17}$ The Heaviside function is often denoted by $H$. However, since this letter is already very much used in transport theory, it is preferred here to use $\Theta$, which is also sometimes used.

[^151]:    ${ }^{18}$ See in particular John P. Church: Spatially dependent integral neutron transport theory for heterogeneous medium using homogeneous Green's functions, thesis from the University of Florida, $\mathrm{n}^{\circ}$ 63-7471, 1963.

[^152]:    ${ }^{19}$ For more on the Dirac delta function, the author recommends (Kanwal 1971, p70) for example.

[^153]:    ${ }^{20}$ For spherical harmonics, the author recommends (Robin 1959).
    ${ }^{21}$ Drew E. Kornreich, Barry D. Ganapol: The Green's function method for nuclear engineering application, Nuclear Science and Engineering, Vol. 126, p293-313 (1997).

[^154]:    ${ }^{22}$ Rudolph Peierls (1907-1995) was an English physicist of German origin. He was born in Berlin in a Jewish family. After studying physics at the University of Berlin, and then that of Munich (with Arnold Sommerfeld), and finally Leipzig, he obtained his PhD in 1929. He then became the assistant of W. Pauli in Zurich. After numerous stays across Europe in different research labs, he obtained in 1933 a fellowship from the Rockefeller Institute and left for England, which would become his home. He found a position at the University of Manchester where he worked on the statistical mechanics of alloys before moving to Cambridge where he worked with P.G.L. Kapur on liquid helium and supraconductivity. He also worked on the theoretical equations for nuclear reaction calculations, from the works of Breit-Wigner. This led to the Kapur-Peierls model. From 1937 to 1963, he was a full Professor at the University of Birmingham, first appointed to the Applied Mathematics Chair (1937-1945), and then to the Mathematical Physic Chair (1945-1963). In March 1940, he co-authored with Frisch the famous memoir on the construction of an atomic bomb from uranium-235. Peierls also contributed to the English team of the Manhattan project. After the war, he returned to Birmingham where he worked on nuclei and nuclear forces models in the quantum physics framework. Laden with honors (Planck medal, Lorentz medal, Dirac medal but surprisingly no Nobel Prize), he was knighted by the Queen of England in 1968. He spent the end of his career at the University of Oxford until 1974.

[^155]:    ${ }^{23}$ J. Chernick: Theory of uranium-water lattices in [Atoms for peace, 1955 Volume V, p243-261].
    ${ }^{24}$ J.R. Askew: Review of the status of collision probability methods, Proceedings of a seminar on numerical reactor calculations held in Vienna by the AIEA, 17-21 January 1972, p185-209 (1972). Askew is one of the main developer of the English code WIMS.

[^156]:    ${ }^{25}$ Some authors well-read in the numerical aspects prefer denoting the probability of first collision in the zone $j$ of a neutron emitted in the zone $i$ by $P_{j i}=P_{j \rightarrow i}$ by respecting the matrix notation row-column which arises in the numerical modeling of the problem. This text being purely theoretical, we have chosen the "frank" notation, which seems more instructive. However, the reader should be very careful about this when reading other reference textbooks.

[^157]:    ${ }^{26}$ William Gee Bickley, John Nayler: A short table of the functions $K i_{n}(x)$ form $n=1$ to $n=16$, Philosophical Magazine Vol. 20, issue 13 pp343-347 (1935).
    ${ }^{27}$ William Gee Bickley (1893-1969) was a British mathematician. After studying mathematics and physics at the University College of Reading, he taught in different schools in Tadcaster, Loughborough and Westminster City. He published his first paper on a hydrodynamics problem, and then became a lecturer at the Battersea Polytechnic in 1919. He became an assistant Professor at the Imperial College in 1930. In 1947, he was made full Professor. He was known for his important work in numerical analysis (such as numerical differentiation equations), on Bessel functions, and he wrote a cornerstone book with G. Temple on the Rayleigh principle. Throughout his life, he had always been mindful of the proper use of applied mathematics to physics.
    ${ }^{28}$ John Nayler. Little is known on Nayler except for his official distinctions: Associate of the City and Guild Institute (of the Imperial College), Bachelor of Science in Engineering, Diploma of Imperial College. It should be noted, however, that his name is often misspelled as Naylor, i.e., with an ' $o$ ', probably owing to an initial typo that has since been reproduced in several neutronic textbooks. The website of the Philosophical Magazine, one of the oldest commercial scientific journals and published by Taylor and Francis continuously since 1798, is categorical on the exact spelling of his name.

[^158]:    ${ }^{29}$ See, for example, R.D.M. Garcia: Collision probabilities in $r-\theta-z$ geometry, Nuclear Science and Engineering, 153, p46-59 (2006).

[^159]:    ${ }^{30}$ Alain Kavenoky: Neptune: un système modulaire pour le calcul des réacteurs à eau légère [Neptune: a modular system for modeling Light Water Reactors], Scientific and Technical Information Bulletin of the $C E A, \mathrm{~N}^{\circ} 212, \mathrm{p} 7-20$ (1976).

[^160]:    ${ }^{31}$ Anne-Marie Brun: Généralisation de la méthode des probabilités de collision pour tenir compte soit du gradient de flux, soit du choc linéairement anisotrope, application au calcul du réacteur Minerve [Generalization of the collision probability method to account either for the flux gradient or a linearly anisotropic collision, and its application to modeling the reactor Minerve], thesis at the University of Orsay (1969).

[^161]:    ${ }^{32}$ R.M. Westfall: Cosine current transmission probabilities for spherical shells, Transactions American Nuclear Society, 18, 147 (1974).
    ${ }^{33}$ E.E. Bende, A.H. Hogenbirk: Analytical calculation of the average Dancoff factor for a fuel kernel in a pebble bed high-temperature reactor, Nuclear Science and Engineering, 133,147-162 (1999).

[^162]:    ${ }^{34}$ M. Segev, G. Raitses, J.M. Paratte: In-rod effective cross sections of resonance absorbers evaluated with routine cell codes, Nuclear Science and Engineering, 131, 123-131 (1999).

[^163]:    ${ }^{35}$ Paul Reuss rightly points out the importance of the assumption of "flat" fluxes (uniform and isotropic) in this calculation. Otherwise, the probability $P_{V S, 0}$ is different from one collision to the other, making the logic of the geometric series meaningless.

[^164]:    ${ }^{36}$ D.L. Henderson, C.W. Maynard: Time-dependent first-flight leakage rates for slabs, spherical shells and spheres, Nuclear Science and Engineering, 97, 203-210 (1987).

[^165]:    ${ }^{37}$ P.M. Keller, J.C. Lee: A time-dependent collision probability for one-dimensional space-time nuclear reactor kinetics, Nuclear Science and Engineering, 129, 124-148 (1998).

[^166]:    ${ }^{38}$ Li Mao: Contribution à la résolution de l'équation de Boltzmann en multigroupe par les mé thodes déterministes et Monte-Carlo [Contribution to the resolution of the Boltzmann equation in multi-group by deterministic and Monte-Carlo methods], thesis at the University of Aix-Marseille (1998). This thesis contains a very complete chapter on the interface current method.

[^167]:    ${ }^{41}$ Pierre Benoist, Alain Kavenoky: La méthode $C_{n}$ de résolution de l'équation du transport: application à la géométrie plane [The $C_{n}$ method for solving the transport equation: application

[^168]:    to a plane geometry], Numerical reactor calculations, Proceedings of a seminar on numerical reactor calculations held in Vienna by the AIEA, 17-21 January 1972, p211-229 (1972).

[^169]:    ${ }^{42}$ On Fourier transforms, the author recommends (Kaplan 1962).

[^170]:    ${ }^{43}$ In $3 D$, the Fourier transform is given by $\int_{0}^{+\infty} f(r) \frac{\sin B r}{B r} 4 \pi r^{2} d r$ and in $2 D, \int_{0}^{+\infty} f(r) J_{0}(B r) 2 \pi r d r$.

[^171]:    ${ }^{44}$ Adnan Ahmad Aswad: A numerical solution to the neutron one-velocity time-independent Boltzmann equation in slab geometry using a homogeneous Green's function and its Pn angular moments, PhD at The University of Florida, 1964.

[^172]:    ${ }^{45}$ José Guasp: The Green's function in the secondary model of thermalization, thesis completed in the science university of Madrid, 1970. Jose Guasp previously obtained an MSc degree in physics at the University of Madrid (Universitas Complutensis, Espagne) in 1961. As from 1962, he worked as a researcher at the "Junta de Energia Nuclear" (the Spanish atomic energy commission, now called CIEMAT) in the theoretical physics field. He became a member of the fusion department of the same CIEMAT (now called the "Asociacion EURATOM/CIEMAT para Fusion"). His fields of interest are the transport equation, the optimization of the stellarator concept, and the heating of neutral particles by lasers. He was on secondment for long periods (including the whole of 1992) in Japan (NIPS in Nagoya) on topics related to plasma physics.

[^173]:    ${ }^{46}$ Dan G. Cacuci: On the slowing down and transport of neutrons in an infinite medium, Nuclear Science and Engineering 108, p50-68 (1991).

[^174]:    ${ }^{47}$ Pierre Lafore (1918-), was an engineer at the CEA who proposed the thesis subject of and supervised Jean-Paul Millot. Born on the 14th of August 1918 and a telecommunications engineer, he was imprisoned for five years during the Second World War. He then worked for seven years as Civil Servant of the State in the Corps (Administration) of Telecommunications in Poitiers, before applying for a position at the CEA, where he was employed on secondment. He worked mainly in Fontenay in the radioprotection field, and studied for a long time the diffusion of neutron in different materials (concrete, graphite, etc.).

[^175]:    (Courtesy Millot family)
    ${ }^{48}$ P. Lafore, J.P. Millot: Etude de l'équation de Boltzmann à une dimension [On the study of the 1D Boltzmann equation], Industries Atomiques (Atomic Industries) n9/10 (1958).

[^176]:    P. Lafore, J.P. Millot: Etude de la diffusion isotrope des neutrons [On the study of isotropic scattering of neutrons], Industries Atomiques [Atomic Industries] n ${ }^{\circ} 5 / 6$ (1959). These two articles, maybe heralding the works of K. M. Case, were published in French in a little-known Swiss vulgarization magazine.
    ${ }^{49}$ Kenneth M. Case, Elementary solutions of the transport equation and their applications, Annals of Physics, Vol. 9 pp1-23, (1960).

[^177]:    ${ }^{50}$ N.G. Van Kampen: On the theory of stationary waves in plasmas, Physica Vol. XXI, pp949-963 (1955).
    ${ }^{51}$ Nicolass "Nico" Godfried Van Kampen (1921-2013). Dutch physicist. He studied theoretical physics at Leiden University under the supervision of Hendrik Krames. His thesis in 1952 dealt with the "contribution of scattering of light to quantum physics". He then worked at Institute for Theoretical Physics at Utrecht University. He is the author of the book "Stochastic processes in physics and chemistry" (1981), which is considered to be the reference in the field.

[^178]:    ${ }^{52}$ Lev Davidovitch Landau (1908-1968). Russian physicist. After studying at Petrograd University, he started a thesis in 1924 at Leningrad State University (which he did not defend!). The Soviet government authorized him in 1929 to go work in European laboratories (Göttingen, Leipzig, Copenhague, Cambridge and Zurich). In 1938, he is imprisoned for a year on the charge of being a spy for the Nazis (!). In 1945, he joined the Science Academy of the USSR without the support of the party because his Jewish origins made him suspicious in the eyes of the communist power in place. In 1949, he started a substantial book with Lifchitz. He was awarded the Nobel Prize in 1962 for his work on condensed states of matter. It was during that year that a very serious car accident put him in a deep coma. While he did come out of it, it did destroy his intellectual abilities.

[^179]:    ${ }^{54}$ Mathematicians instead talk of the discrete spectrum of a linear operator (Dowson 1978), which meant that Case's theory was looked upon with caution in the beginning. Paul Zweifel, probably due to an unfamiliarity with the works of Lafore and Millot of 1958, remarked that it was only in 1988 that Case's approach was finally rigorously mathematically validated. The works of Paul Zweifel in neutronics are authoritative. After a Ph.D. at Duke University in 1954, he worked in the theoretical division of Knolls Laboratories. In 1958, he started teaching at the University of Michigan-which he would do for ten years. It is also where he would work with Kenneth Case, with whom, he would write the very famous "Linear Transport Theory", one of the most important texts in neutronics. In 1968, he became a Professor at Virginia Tech, where he would remain until his retirement in 1996.

[^180]:    ${ }^{56}$ Ivar Fredholm (1886-1927) was a Swedish mathematician who distinguished himself in the study of integral equations and the use of spectral theory. He defended his thesis in 1898 at Uppsala University. He studied in France the Dirichlet problem, for which he put forward a new integral approach. Dead before the discovery of the neutron, his work in applied mathematics remains very useful in this branch of physics.

[^181]:    ${ }^{60}$ Noel R. Corngold (1929-). After an undergraduate degree at Columbia in 1949, this American theoretical physicist completed an experimental Ph.D. at Harvard in 1954. He was then sent to Brookhaven National Laboratory to carry out an accurate measurement of the magnetic moment of the neutron. He specialized in neutronics there. He then joined Caltech in 1966 to work in the nuclear engineering department. As from 1966, he took a special interest in the dynamics of systems with a large number of particles, in particular the plasmas of the small tokamak built by Roy Gould at Caltech. He taught applied physics at Caltech from 1966 to 2002. Corngold won the Wigner medal in 2002 for his theoretical work in neutronics.

[^182]:    ${ }^{61}$ In particular, Clarence Lee, in his very complete report in the $\mathrm{S}_{\mathrm{n}}$ method: The discrete $S_{n}$ approximation to transport theory, Los Alamos Scientific Laboratory, LA-2595, 200 pages (1962), used the same definition of the angle $\theta$ in spherical and cylindrical coordinates. It should be noted that his $\phi$ is our $\theta$.

[^183]:    ${ }^{1}$ Bengt G. Carlson: Solution of the transport equation by $S_{n}$ approximations, Los Alamos, report LA-1599, (1953). Carlson (1916-2007) was a civil scientist in the Manhattan project as from 1943 for the English mission in Canada. In June 1945, he was transferred to Los Alamos National Laboratory to perform numerical calculations on the bomb. He retired from the Theory division in 1976. For 10 years, he has continuously improved the discrete ordinates method. The initial idea is from G. C. Wick (1943) (Stamm'ler and Abbate 1983, p. 209), but it was S. Chandrasekhar who developed the principle in his renowned work Radiative transfer, Oxford (1950). The work of Carlson, Lee and Lathrop has been essential to set up efficient quadratures which minimize the number of directions in the discrete problem. According to K. D. Lathrop, the ray effect in the 2D method has been observed in the middle of the 1960's. This effect can be solved by adding an angular source which adds up to zero and which transforms the discrete ordinates equations into spherical harmonics equations. For the short story, Carlson wanted to underline the major role played by Stanley Ulam in the development of the H-bomb compared to the (irritating and criticized) Edward Teller in an interesting article: How Ulam set the stage, Bulletin of Atomic Scientists, vol. 59, no. 4 (2003).
    ${ }^{2}$ Clarence E. Lee: The discrete $S_{n}$ approximations to transport theory, Los Alamos scientific laboratory, LA-2595 (March 1962).
    ${ }^{3}$ D.K. Trubey, Betty F. Maskewitz: A review of the discrete ordinates $S_{n}$ method for radiation transport calculations, Oak Ridge National Laboratory ORNL-RISC-19 (March 1968) presents a set of applications, including a theoretical text of Carlson himself.

[^184]:    ${ }^{4}$ K.D. Lathrop: Ray effects in discrete ordinate equations, Nuclear Science and Engineering, no. 32, p. 357 (1968).

[^185]:    ${ }^{5}$ Adrien-Marie Le Gendre (1762-1833) was a brilliant French mathematician of whose life little is known. His name is often spelt Legendre, which will be used throughout this work, although not appropriate. The polynomial basis that bears his name is very useful for its orthogonal properties. On a side note, it was only in 2008 that a plausible portrait of Legendre was found-until then, he was confused with Louis Legendre, Montagnard during the French Revolution.

[^186]:    ${ }^{6}$ In the paper The early days of the $S_{n}$ method, ANS transaction, vol. 66, pp. 241-242 (1992), K. D. Lathrop uses the term Angular Segmentation for the origin of the term $S_{n}$.

[^187]:    ${ }^{7}$ A. Takahashi et al., Journal of Nuclear Sciences and Technology, 16, 1, 1 (1979). The NITRAN code distributed by OECD is based on this method.

[^188]:    ${ }^{8}$ Jacques Ligou, Patrick Miazza: Numerical improvements of the exact kernel method in transport theory, Nuclear Science and Engineering, 99, pp. 109-117 (1988).
    ${ }^{9}$ The main property of the Legendre polynomials is that they are orthogonal by integration $[-1$, $+1]$. For orthogonal functions, (Sansone 1959) constitutes an excellent reference work.

[^189]:    ${ }^{10}$ It should be remarked that some authors (including the French school (Bussac and Reuss 1985), Pierre Benoist, and logically the $C E A$ code APOLLO2) include the $(2 l+1)$ coefficient in the flux

[^190]:    ${ }^{11}$ R.E. Marchak, A note on the spherical harmonic method applied to the Milne problem for a sphere, Phys. Rev. 71, no. 7, 443 (1947).

[^191]:    ${ }^{12}$ J. Ligou, J. Stepanek, P.A. Thomi: Forme intégrale de l'équation du transport, approximations polynomiales et diffusion isotrope [Integral form of the transport equation, polynomial approximations and isotropic scattering], Proceedings of a seminar on numerical reactor calculations held in Vienna by the AIEA, 17-21 January 1972, pp. 231-265 (1972).

[^192]:    ${ }^{13}$ E. M. Gelbard: Simplified spherical harmonics equations and their use in shielding problems, Westinghouse report WAPD-T-1182, (1961).Ely Gelbard (1924-2002) studied in New York at Evander Childs High School (1942), then at the University of Pittsburgh. He held a PhD in physics at the University of Chicago. During his 50 -year career, he initially worked at Bettis before moving to the applied physics division of Argonne National Laboratory where he developed and improved several calculation methods in reactor physics, especially the $S P_{n}$ method in 1961 or the synthetic method applied to $S_{n}$ equations in 1969. He also worked on the Monte Carlo method, his work in that field culminating in the co-authoring of (Spanier and Gelbard 1969). He received the Ernest Lawrence Prize in 1969 for his contribution to numerical methods in reactor physics and the Wigner Medal in 1995.

[^193]:    ${ }^{14}$ E.W. Larsen, J.M. McGhee and J.E. Morel: The Simplified PN Equations as an Asymptotic Limit of the Transport Equation, Transactions of American Nuclear Society, 66, 231 (1992). Edward W. Larsen (1944-) defended his PhD thesis in 1971 (Completeness Results for Linear Operators in a Hilbert Space and Problems in Neutron Transport Theory) at the Rensselaer Polytechnic Institute of Troy (New-York). He teaches at the department of nuclear engineering of the University of Michigan at Ann Arbor. His research areas include the transport equation and mathematical models in neutron physics. He has obtained several awards among which the Arthur Holly Compton Award of the ANS in 1996. He has authored or co-authored almost 300 papers, most of which are on the transport equation, thereby making him one of the rare international specialists in the field.

[^194]:    Edward Larsen (1944-) Courtesy Larsen

[^195]:    ${ }^{16}$ Gerald C. Pomraning (1936-1999) completed his PhD in nuclear engineering at the MIT in 1962. He worked for 7 years at General Electric and at General Atomics, and then helped in founding in 1969 the services company Science Applications International Corporation based in San Diego. SAIC and its subsidiaries now employ more than 35,000 persons worldwide. In 1978, he joined UCLA where his research areas were the transport equation, reactor kinetics and nuclear reactor at large. He encompasses both the fields of physics and applied mathematics very elegantly. He received several awards such as the Wigner Medal in 1999, and participated actively to journals in the field: Nuclear Science and Engineering and Transport Theory and Statistical Physics. ANS created an award that bears his name: The Gerald C. Pomraning Memorial Award, which was attributed to Richard Sanchez from CEA in 2009. "Jerry" Pomraning has written several high standard papers on neutron transport, but cancer took him too early. He will be remembered as somebody who loved life, and enjoyed good food and cigars.

[^196]:    (Courtesy Pomraning)
    ${ }^{17}$ Alain Hébert: The search for superconvergence in spherical harmonics approximations, Nuclear Science and Engineering, 154, pp. 134-173 (2006).

[^197]:    ${ }^{18}$ Jones (1985) is a complete reference for proofs on the use of spherical harmonics in field theory.
    ${ }^{19}$ Eugenio Beltrami (1835-1900) was an Italian mathematician and physicist who worked in both the fields of mathematics (differential geometry and non-Euclidean geometry) and physics (optics, thermodynamics, electromagnetism-a subject area where he introduced the modified Laplace operator). He held the position of professor in several Italian universities and was appointed president of the prestigious Accademia dei Lincei in 1898.

[^198]:    ${ }^{20}$ See in particular J. K. Fletcher: The solution of the multi-group neutron transport equation using spherical harmonics, Nuclear Science and Engineering, 84, pp. 33-46 (1983).

[^199]:    ${ }^{21}$ Edward Arthur Milne (1896-1950) was a British mathematician and astrophysicist. Following his degree in Cambridge in 1914, he started working as the assistant director of the sun physics observatory. He taught applied mathematics at the University of Manchester from 1924 to 1928 then was awarded the mathematics chair at Oxford. Milne is particularly well-known for his work in astrophysics where he proposed an expansion model for the universe which is different from Einstein's: he introduced a heterogeneous universe density that changes over time-this theory is presently disproved by measurements.

[^200]:    ${ }^{22}$ M. Trocheris, C. Mercier, J. Yvon: Sur la répartition angulaire des vitesses des neutrons thermiques dans un milieu hétérogène [On the angular distribution of thermal neutron speeds in a heterogeneous medium], physics seminar at Bologna, 2 pages (September 1950), a summary of which is given in (Yvon 1985, p. 487).
    ${ }^{23} \mathrm{~J}$. Yvon: La diffusion macroscopique des neutrons, une méthode d'approximation [Macroscopic neutron scattering, an approximation method], Journal of Nuclear Energy, 1, 4, 305 (1957). Jacques Yvon (1903-1979) was a famous French physicist. After his studies at the Ecole Normale Supérieure, where he obtained the physics aggregation, he became a lecturer at the University of Strasbourg in 1938. During the war, he was deported to Germany in 1943. After the war, he joined the CEA in 1949. He was the first head of the mathematical physics service, the precursor of the present-day SERMA, before becoming head of the reactor studies department (1952), and director of the physics of the atomic piles (1959-1962). During that period, he was one the main actors of the French graphite-gas reactors. In 1962, he returned to a university career as professor of theoretical physics at the Faculty of Sciences of Paris. Afterwards, he was appointed the high

[^201]:    ${ }^{24} \mathrm{~A}$ complete history of the transport theory and the contributions of K. M. Case may be obtained in P.F. Zweifel: Transport theory revisited, Transport Theory and Statistical Physics, 26 (1\&2), pp. 181-193 (2007).

[^202]:    ${ }^{25}$ Refer to Dowson (1978) for fundamentals on the spectrum of a linear operator.

[^203]:    ${ }^{26}$ B. Ganapol, J.C. Garth, S. Woolf: Analytical neutral particle benchmark in half-space geometry, proceedings of Conference on Mathematical methods and supercomputing in nuclear applications, Karlsruhe, 1993, Vol. 2, pp. 284-295. Barry Ganapol (1944-) is a renowned American specialist of the transport equation in neutron physics. After a PhD in physics at Berkeley in 1971 on the Time dependent neutron transport theory, he works in several international laboratories in the nuclear field: the Swiss Federal Institute for Reactor Research, the CEA Saclay from 1972 to 1974 and the Weizmann institute in Israel. Since 1976, he has been a professor at the University of Arizona at the department of aerospace and mechanical engineering. He specialized in numerical methods applied to neutron physics.

[^204]:    ${ }^{27}$ Subrahmanyan Chandrasekhar (1910-1995) was an astrophysicist of Indian origin. After his studies at Madras, in 1933, he read his PhD in England at Trinity College, Cambridge. Afterwards, he worked on stellar astrophysics and the radiative emission and plasma problems. He is wellknown for having determined the time at which a white dwarf collapses into itself (Chandrasekhar limit). In 1937, he immigrates to the United States where he teaches at the University of Chicago. In 1983, he was awarded the Physics Nobel Prize. For our subject matter, his book on radiative transfer (1960) is the most suited.

[^205]:    ${ }^{29}$ Refer to Nixon (1964) for Laplace transforms.

[^206]:    ${ }^{30}$ In mathematics, the Heaviside step function is denoted as H , but $\Theta$ is used here to avoid any confusion with the Chandrasekhar function. The Laplace transform of $\Theta$ is $1 / p$.
    ${ }^{31}$ This kernel contains the probability that was denoted $N(u)$ in the chapter on slowing-down.

[^207]:    ${ }^{32} \ln \left(\frac{1+x}{1-x}\right)=2 \operatorname{Arg} \tanh (x), \ln \left(\frac{1+i x}{1-i x}\right)=2 i \operatorname{Arg} \tan (x)$

[^208]:    ${ }^{33}$ R. Roy, A. Hébert, G. Marleau: Consistent $B_{n}$ theory for slab lattices, Nuclear Science and Engineering 115, pp. 112-128 (1993).

[^209]:    ${ }^{34}$ M.S. Milgram: The method of the ultraspherical harmonics in particle transport, ANS Proc. Advances on nuclear engineering computation and radiation shielding, Santa Fe (1989).

[^210]:    ${ }^{35}$ B.D. Ganapol: A neutron transport benchmark in one-dimensional cylindrical geometry: revisited, Nuclear Science and Engineering, 159, pp. 169-181 (2008).

[^211]:    ${ }^{36}$ Théo Kahan (1904-1984) was a French physicist and pioneered the development of theoretical methods in quantum physics and electrodynamics. With Raymond Jancel (1926-2011), he created a research team in mathematical physics at the Institut Henri Poincaré at La Sorbonne, Paris, where he taught for several years. He is the author of many books on modern physics as well as several works for popularizing physics (among which a Que. sais-je [What do I know] edition on atomic structure and another one on radio waves) and one of the first textbooks on reactor physics in French (Kahan and Gauzit 1957). He is also the co-author of a book with Jancel on plasma electrodynamics which has been translated to English in 1966 by the publishing company, John Wiley. He was said to be close to Frédéric Joliot with whom he had common political views.
    ${ }^{37}$ T. Kahan, G. Rideau: Sur la déduction de divers principes variationnels de la théorie des collisions à partir d'un principe unique [On the deduction of various variational principles of collision theory from a single principle], Journal de Physique du Radium, 13, p. 326 (1952). Also refer to (Kahan et al. 1956).

[^212]:    ${ }^{38}$ Historically, Kavenoky defined the $C_{n}$ approximation as a truncated Taylor expansion at order $n-1: \Phi(\mu)=\sum_{l=1}^{n} \Phi_{l} \mu^{l-1}$, which did not seem very wise to us for comparison with the $P_{n}$ or $T_{n}$ methods, as well as for the numbering of the moments. Nevertheless, the principles remain the same.

[^213]:    ${ }^{39}$ Alain Kavenoky, Henri Lorain: Théorie de l'expérience exponentielle: application de la mé thode $C_{n}$ et des modèles synthétiques de ralentissement [Theory of the exponential experiment: application to the $C_{n}$ method and synthetic slowing-down models], technical note CEA-N-1582 (1973).
    ${ }^{40}$ Henri Lorain, Modèles synthétiques de ralentissement des neutrons et méthode $C_{n}$ : application à l'interprétation des expériences exponentielles rapides [Synthetic neutron slowing-down models and the $C_{n}$ method: interpretation of fast exponential experiments], PhD thesis, University of Orsay (1972).
    ${ }^{41}$ Pierre Benoist, Alain Kavenoky, Henri Lorain: The $C_{n}$ method of approximating Boltzmann equation and fast exponential problems, transactions of American Nuclear society, 14, p. 224 (1970).
    ${ }^{42}$ M. Krook, On the solution of equations of transfer, Astrophysics Journal 122, p. 488 (1955).
    ${ }^{43}$ Bernard I. Spinrad, J. S. Sterbentz, Approximations to neutron transport problems in complex geometries, Nuclear Science and Engineering 90, pp. 431-440 (1985).
    ${ }^{44}$ Zekeriya Altaç, Bernard I. Spinrad, The $S K_{n}$ method I: a high-order transport approximation to neutron transport problems, Nuclear Science and Engineering 106, pp. 471-479 (1990).

[^214]:    ${ }^{45}$ Bernard I. Spinrad, Zekeriya AltaÇ, The $S K_{n}$ method II: heterogeneous problems, Nuclear Science and Engineering 106, pp. 480-488 (1990).

[^215]:    ${ }^{46}$ François Févotte: Techniques de traçage pour la méthode des caractéristiques appliquée à la ré solution de l'équation du transport des neutrons en domaines multidimensionnels [Tracing methods for the method of characteristics applied to the resolution of the transport equation in multidimensional domains], PhD thesis, Paris, 2008.

[^216]:    ${ }^{47}$ As defined by Robert Roy: The cyclic characteristics method, International Conference on the Physics of Nuclear Science and Technology, Long Island, USA, October 1998, pp. 407-414 (1998).

[^217]:    ${ }^{48}$ Richard Sanchez, Li Mao, S. Santandrea: Treatment of boundary condition in trajectory-based deterministic transport methods, Nuclear Science and Engineering, 140, pp. 23-50 (2002).
    ${ }^{49}$ M. Assawaroongruengchot, Guy Marleau: Multi-group adjoint transport solution using the model of cyclic characteristics, Nuclear Science and Engineering, 155, pp. 37-52 (2007).

[^218]:    ${ }^{50}$ S.G. Hong, N.Z. Cho: Method of characteristic direction probabilities for heterogeneous lattice calculation, Nuclear Science and Engineering 132, pp. 65-77 (1999).

[^219]:    ${ }^{51}$ Jean-Michel Ruggieri: Méthodes numériques pour la prise en compte d'hétérogénéités locales dans les calculs neutroniques de cours de réacteurs [Numerical methods to allow for local heterogeneities in the calculation of nuclear reactor cores], PhD thesis, University of Provence (1995). This thesis discusses the even-parity flux.
    ${ }^{52}$ Daniel Verwaerde (1954-). After engineering studies at Ecole Centrale Paris (1977), he joined the Department of Applied Mathematics of the CEA/Direction of Military Applications in 1978. He developed during 10 years programs for particle transport with the Boltzmann equation. His works on several topics in numerical methods are worth noting: numerical methods with finite differences and finite volumes for the cylindrical transport equation (DSN methods), acceleration of convergence of algorithms with the "Fine mesh rebalancing" method or the Diffusion Synthetic Acceleration, the collisionless flux methods, or discrete ordinates methods based on LobattoChebychev quadrature, discontinuous finite element methods for transport equations for which the solution may have significant local variations, the probability method for neutron chain when the number of neutrons is weak (Hansen), the setting up of probability equation for $n$ neutrons ( 0 to large numbers), the adjoint approach for the Boltzmann equation. His more significant contributions include the even-parity equation, the original variational formulations and the existence of the solutions based on the Lax-Milgram lemma and the generalized Poincaré inequality proof, the asymptotic behavior of the even flux in the diffusion equation as well as the construction of numerical methods for continuous finite elements compatible with the even flux and the diffusion. This list proves the extent of contributions in neutron transport. He was appointed as director of the Department of Applied Mathematics in 1986. In 1996, he became director of the Simulation

[^220]:    (Courtesy Verwaerde)
    ${ }^{53}$ Only the isotropic case has been illustrated here, but the PhD thesis of Bruno Ackherraz describes the derivation for anisotropic cases: Anisotropie du choc en transport des neutrons par la méthode des éléments finis primaux [Anisotropy in neutron transport for the method of primal finite elements], PhD thesis, University of Pierre and Marie Curie-Paris VI (1995).

[^221]:    ${ }^{54}$ D. Verwaerde: Les approximations déterministes de l'équation du transport des neutrons [Deterministic approximation of the neutron transport equation], CHOCS no. 4, pp. 37-44, CEA/DAM magazine, (December 1991).

[^222]:    ${ }^{55}$ R.T. Ackroyd: Foundations of finite element applications to neutron transport, progress in nuclear energy, Vol. 29, no. 1, pp. 43-56 (1995).

[^223]:    ${ }^{56}$ Especially the works of E.E. Lewis and I. Dilber: Nucl. Sci. Eng. 91, 45 (1985) and Progr. Nucl. Energy 18, 63 (1986).
    ${ }^{57}$ V.S. Vladimirov: Transactions V.A. Steklov Mathematical Institute, 61 (1961) in Russian. An English translation can be found in: Mathematical problems in the one-velocity theory of particle transport, Atomic Energy of Canada, (1963).
    ${ }^{58}$ Vassili S. Vladimirov (1923-2012) was a Russian mathematician. He was a pioneer in the analysis of complex multivariate functions and the author of a mathematical textbook for physics. He contributed to the development of the Russian atomic bomb. Furthermore, he was also a member of the USSR Academy of Sciences as of 1970 and was awarded the Stalin Medal in 1953, as well as several military awards for the part he played in World War II.

[^224]:    ${ }^{59}$ R.T. Ackroyd, C.R.E. de Oliveira: A variational treatment for the time dependent Boltzmann equation as a basis for numerical conserving neutrons, Progress in Nuclear Energy Vol. 30, no. 4, pp. 417-465 (1996).

[^225]:    ${ }^{60}$ Jean-Claude Nimal. After Ecole Centrale Paris, he obtained a PhD and spent his whole career at the CEA/SERMA where he was in charge of the group for the Monte Carlo code (TRIPOLI), fuel cycle codes (PEPIN, FAKIR) or radioprotection codes (MERCURE, SN1D, etc.). He was appointed Director of Research in recognition of his expertise.
    ${ }^{61}$ Jean Rastoin (1932-2009). After Ecole Polytechnique (admitted in 1951), he chose naval engineering. He worked as engineer for naval constructions and weaponry (1956-1962), and was detached at the CEA (since 1958). He was successively deputy chief of the pile radioprotection studies (1962-1970), head of service (1970-1975) and head of the department of mechanical and thermal studies (1975-1982). Furthermore, he was also director of studies and reactor conception (1983-1990) and administrator of the center for technical studies for mechanical industries (CETIM in French) (1977-1980), of Sofretes (1979-1983) and Aerowatt (1980-1985). Later on, he was appointed director of the Institute for protection and nuclear safety (IPSN) (1990-1991), vice-president of the institute of electronics of Paris, and the Sociéte française des mécaniciens (SFM—French Society of Mechanical Engineers) (since 1996).

[^226]:    ${ }^{63}$ The mathematical expectation of a game with discrete values $X_{i=1, n}$ with probability $p_{i=1, n}$ is equal to $E(x)=\sum_{i=1}^{n} p_{i} X_{i}$. Hence, the expectation of a non-biased dice with six equiprobable indexed faces $(p=1 / 6)$ is $E(X)=(1+2+3+4+5+6) / 6=3.5$. For a continuous variable: $E$ $(X)=\int p(X) X d X$.

[^227]:    ${ }^{64}$ For example: B. Morillon: Méthode de Monte-Carlo non analogue, application à la simulation des neutrons [Non-analogue Monte Carlo method applied to neutron simulation], PhD thesis, Paris, January 1996.

[^228]:    ${ }^{65}$ Jean Gonnord (1947-): Etude de phénomènes de thermalisation par la méthode de Monte-Carlo. Application au calcul de l'absorption des neutrons par des poisons consommables dans les ré acteurs à eau légère [Study of thermalization phenomena using the Monte Carlo method. Application to the calculation of neutron absorption by burnable poisons in light water reactors], PhD thesis from University of Orsay (1973). Jean Gonnord obtained an engineering degree from ESPCI (physics and chemical engineering school from Paris) and a PhD in atomic physics. He joined the CEA in 1973 at the Direction of Reactor Studies where he worked on Monte Carlo, and then moved to the Direction of Military Applications (DAM in French) after working in robotics. He led the simulation project at CEA/DAM where he headed the TERA project in particular which saw the upcoming of the TERA-10 computing machine from BULL, the fifth computer in the world ranking and first in Europe in 2005. Later on, he worked on the TERA1000, the first petaflop computer in Europe, conceived as partnership between CEA and BULL. Jean Gonnord is an international expert in the fields of mathematics, information, programming and system technologies at CEA.

[^229]:    ${ }^{66}$ From the work of R. Eyraud: Calcul de l'absorption épithermique dans les réseaux plans irré guliers par la méthode de Monte-Carlo [Calculation of epithermal absorption in lattices with irregular planes using the Monte Carlo method], Paris, 1967.

[^230]:    ${ }^{67}$ S. Cramer: Derivations of the solid angle subtended at a point by first- and second-order surfaces and volumes as a function of elliptic integrals, Nuclear Science and Engineering, 132, pp. 217-258 (1999).

[^231]:    ${ }^{68}$ For directional biasing, refer to R.P. Gardner, M. Mickael, K. Verghese: A new direction biasing approach for Monte-Carlo simulation, Nuclear Science and Engineering, 98, pp. 51-63 (1988).

[^232]:    ${ }^{69}$ For the use of deterministic-stochastic coupling using the deterministic adjoint flux to accelerate non-analogue simulations, refer to the PhD thesis of François-Xavier Giffard: Développements utilisant des méthodes stochastiques et déterministes pour l'analyse de systèmes nucléaires complexes [Developments using the stochastic and deterministic methods for analyzing complex nuclear systems], PhD thesis, University of Evry (2000).
    ${ }^{70}$ Régis Eyraud (1940-). After his engineering studies at Ecole Centrale de Paris (1964) and Master's degree in mathematics (1965), he completed a PhD at the CEA/SERMA where he developed the first French Monte Carlo code: CARPE, the precursor of the TRIPOLI code. He worked at the CEA until 1970, then joined Schlumberger to work on real-time information technology. He joined the MATRA group in 1971 up to 1993 and read an MBA at HEC in 1980 (operational research, managing information technology and telecommunications). In 1993, he founded a company for financing capital goods.

[^233]:    ${ }^{71}$ I.V. Serov, T.M. John, J.E. Hoogenboom: A midway forward-adjoint coupling method for neutron and photon Monte-Carlo transport, Nuclear Science and Engineering, 133, pp. 55-72 (1999).
    ${ }^{72}$ The practical implementations of which are illustrated in J.E. Hoogenboom: Application of the midway Monte-Carlo method to nuclear bore hole logging, International Conference on the Physics of Nuclear Science and Technology, Long Island, USA, October 1998, pp. 168-173.

[^234]:    ${ }^{73}$ Thomas E. Booth: A quasi-deterministic approximation of the Monte-Carlo importance function, Nuclear Science and Engineering 104, pp. 374-384 (1990).

[^235]:    ${ }^{1}$ Robert P. Rulko, D. Tomalevic and E.W. Larsen: Variational $P_{1}$ approximations of generalgeometry multigroup transport problems, Nuclear Science and Engineering, 121, p393-404 (1995).

[^236]:    ${ }^{2}$ By convention, products with adjoint flux will be described by notations used solely for that method, i.e. the cross sections at the right of the reaction rate.

[^237]:    ${ }^{3}$ It must be noted that neutrons are not produced in the same place. This reasoning is valid only for space since $k_{\infty}$ is an average value for the reactor, and applies to any point inside it.
    ${ }^{4}$ Roger Naudet: Etude de la migration des neutrons dans un milieu multiplicateur en fonction de l'intensité et de la distribution des captures [Study of neutron migration in a multiplying medium as a function of the intensity and distribution of capture], CEA Report R2476 (1964).

[^238]:    ${ }^{5}$ For fast neutrons, the scattering length $L$ is substituted by the migration path $M$.

[^239]:    ${ }^{6}$ Alain Checroun: Les sources ponctuelles de l'équation de Helmholtz en coordonnées sphériques, journal from CETHEDEC, 5th year, 1st term 1968, No 13, pp. 9-45. The mathematical background is carried out for the Helmholtz equation of type $\Delta \Phi(r, \theta, \varphi)+k^{2} \Phi(r, \theta, \varphi)=0$, a situation that is obtained for multiplying media. Alain Checroun was an assistant at the Faculty of Sciences at Rouen, and a student of Maurice Bouix, professor at the same faculty. Bouix is the author of numerous works on the analytical treatment of the sources of the Maxwell equation and the use of distributions in electromagnetism.

[^240]:    ${ }^{7}$ Alexei Dmitrievitch Galanin (1918-1999) was a Russian physicist. He worked in the group under Pomerantchuk at ITEP. He also worked on field theory and is the author of three reference manuals, one of which is on reactor physics and dates from 1960.
    ${ }^{8}$ In (Galanin 1960), $\gamma_{G}$ has dimensions of [ $\mathrm{cm} / \mathrm{s}$ ] and appears in the diffusion equation for the neutron concentration. In the flux equation, $\gamma$ is dimensionless and is equal to $\gamma_{G} / v$.

[^241]:    ${ }^{9}$ J.S. Cassel and M.M.R. Williams: The thermal diffusion length problem in an array of plates, Nuclear Science and Engineering: 148, 453-457 (2004).

[^242]:    ${ }^{10}$ M. Sagot, G. Cuny and al: MARIUS - HECEMSAC: Mesure de la longueur de diffusion du graphite en expériences exponentielles [Measure of graphite scattering-length in exponential experiments], report SECMG No 29, August 1966, Nuclear Studies Center of Cadarache.

[^243]:    ${ }^{11}$ Manley, Haworth, Lubke, The mean life of neutron in water and the hydrogen capture crosssection, Physical review 61, 152 (1942).

[^244]:    ${ }^{12}$ Franck D. Judge: Neutron transport theory in pulsed multiplying assemblies, PhD at The Renselaer Polytechnic Institute, august 1963.
    ${ }^{13}$ J. Lehner, G.M. Wing, On the spectrum of an asymmetric operator arising in the transport theory of neutrons, Communications on Pure Applied Mathematics Vol. 8, pp217-234 (1955).
    ${ }^{14}$ J. Lehner, G.M. Wing, Solution of the linearized Boltzmann equation for the slab geometry, Duke Mathematical Journal Vol. 23, pp125-142 (1956).
    ${ }^{15}$ S. Albertoni, B. Montagnini, Some spectral properties of the transport equation and their relevance to the theory of pulsed neutron experiments, Pulsed Neutron Research, Proceedings of a symposium, Karlsruhe, 10-14 May 1965, Volume 1, pp239-272.

[^245]:    ${ }^{16}$ Some authors simply call this the diffusion coefficient, but adding the term asymptotic avoids confusion.

[^246]:    ${ }^{17}$ K.H. Beckurts, Review of pulsed neutron experiments, Pulsed Neutron Research, proceedings of a symposium, Karlsruhe, 10-14 May 1965, Volume 1, pp3-34.

[^247]:    ${ }^{18}$ Gérard Cuny (1936-?). After his BSc at Marseille, he was part of the first group of MSc students in Reactor Physics in 1962. Later, for his PhD, he worked at the CEA in the team of Proserpine at the Service for critical experiments of CEA/Saclay of D. Breton. In 1965, he was the co-author of a collective work on the analysis of graphite and beryllium oxide by pulsed neutrons. Paul Reuss indicates that Gérard Cuny passed away at a young age but supplies no further information.
    ${ }^{19}$ G. Cuny, V. Deniz, J. Lalande, J.G. Le Ho and M. Sagot, Etude du graphite et de l'oxyde de beryllium par la method de la source pulse de neutrons, [A study of graphite and beryllium oxide using the neutron pulse source method], Pulsed Neutron Research, Proceedings of a symposium, Karlsruhe, May 10-14, 1965, Volume 1, pp89-104.

[^248]:    ${ }^{20}$ Assuming that the slowing-down law is uniform with energy, Paul Reuss points out that the probability of a neutron dropping straight from 10 MeV to below 0.625 MeV is $\Delta E / E_{0}=0.625 / 10^{7}$, which is negligible.

[^249]:    ${ }^{21}$ Mihran J. Ohonian: Eigenfunction analysis of hydrogeneous neutron spectra, PhD from the Rensselaer Polytechnic Institute, Troy, New York, USA (1963).

[^250]:    ${ }^{22}$ From the work of Michel Tommy-Martin (EDF, 2005).

[^251]:    ${ }^{1}$ Richard Sanchez: An analysis of the stochasticity of the transport equation, Transport Theory and Statistical Physics, volume 26 (4 and 5), 469-505 (1997). Richard Sanchez (1946-) studied at the Polytechnic School of Barcelona. He completed his PhD at the CEA/SERMA [CEA/Department of Reactors and Applied Mathematics] in 1974, which was followed by a higher doctorate in 1974. He subsequently worked for 5 years at the University of Seattle in the United States, and obtained a further PhD in Nuclear Engineering at the University of Washington in 1981. His PhD in 1979 at CEA/SERMA [Schémas approchés de résolution de l'Equation intégrale du transport à deux dimensions (Approximate schemes for the solving of the integral transport equation in two dimensions)] shows his expertise in the field of numerical models in neutron physics. He was behind several improvements of the APOLLO2 code, and is a worldwide expert in transport theory; he has authored more than fifty papers in prestigious professional journals such as Nuclear Science and Engineering or Transport Theory and Statistical Physics, making him the most renowned French neutron scientist at international level. In 2002, he was appointed Director of Research at CEA where he supervised more than twenty doctorates in the transport theory field. He is also associate professor at the Georgia Institute of Technology. Thanks to his proverbial speed of speech and his exceptional character, he is one of the most outstanding figures in French neutron physics.

[^252]:    ${ }^{2}$ Gordon E. Hansen: American physicist who worked at Los Alamos during the 2nd World War. His work on nuclear bomb ignition became famous through the Hansen equation. He wrote many interesting papers in literature relative to criticality. He further married Marian Konopinski, the sister of Emil John Konopinski, the famous specialist of the beta decay.
    ${ }^{3}$ By definition, a generation involves the loss of the generating neutrons, but the same reasoning may be followed in considering a collision (the generation time is the time between two collisions). In this case, scattering should be viewed as a process that produces a new neutron, just like a fission that produces only one neutron, and the number $\bar{m}$ coincides with the definition of $c$ secondary neutrons as seen previously, i.e. the number of neutrons produced by collision. In this second approach, the probability of sterile capture $P_{1,0}(1) \equiv \Sigma_{c} / \Sigma_{t}$ can be computed, as well as the probabilities of fertile captures $P_{1,1}(1) \equiv\left(\Sigma_{s}+p(1) \Sigma_{f}\right) / \Sigma_{t}, P_{1, m \geq 2}(1) \equiv p(m) \Sigma_{f} / \Sigma_{t}$, where $p(m)$ is the probability of emission of $m$ neutrons by fission, as seen in Chap. 2.

[^253]:    ${ }^{4}$ See for example (Blaquière 1962).

[^254]:    ${ }^{5}$ Eugène C. Critoph (1929-1966). B.A.S., M.A.Sc. (British Columbia) joined Atomic Energy of Canada Ltd (AECL) in 1953 and worked in the reactor physics field till 1967. He took on several responsibilities at the Chalk River laboratories, becoming director of the Fuel and Material branch, then director of Reactor Physics and advanced products, and later Vice-President of AECL's Strategic Technology Research Management. Further, in 1986, he was awarded the W. B. Lewis medal by the Canadian Nuclear Association for his extremely extensive research work. He supervised an excellent book: Canada Enters the Nuclear Age, published in 1997, which recounts the history of AECL. On a more personal note, he was believed to be extremely interested in games and puzzles of all types.

[^255]:    ${ }^{6}$ For details on the physics of the MOX fuel, refer to Paul Reuss: Etude physique du recyclage du plutonium dans les réacteurs à eau [Physical studies of the recycling of plutonium in water reactors], PhD thesis (1979) and CEA technical report CEA-N-2098.

[^256]:    ${ }^{7}$ Fuel pin diameter: 0.82 cm , zirconium cladding diameter: 0.92 cm , lattice pitch filled with water at $305^{\circ} \mathrm{C}$ : 1.26 cm , calculated using the Wigner-Seitz method with zero-buckling.

[^257]:    ${ }^{8}$ Dominique Akl: Modèle du réacteur réduit pour le calcul de la variation du flux et de la réactivité résultant d'une perturbation localisée dans un milieu multiplicateur à neutrons rapides [Reduced reactor model for calculating the flux variation and the resulting reactivity for a perturbation in a fast-neutron multiplying medium], PhD thesis, University of Orsay (1972). Perturbation theory is extensively used in this thesis.

[^258]:    ${ }^{1}$ Hermann Ludwig Ferdinand von Helmholtz (1821-1894). After starting out as a military doctor, then an anatomy professor, he became a professor of physics at the University of Berlin. He then worked on experiments in the field of electrophysiology (measurement of the nervous influx), optics and acoustics. He is famous for his definition of potential energy.

[^259]:    Hermann Von Helmholtz (Public domain)

[^260]:    ${ }^{2}$ For a quick primer on Bessel functions, refer to (Harper 1976, p. 186).

[^261]:    ${ }^{3}$ Viktor Amaszaspovitch Ambartsumian, Reports from the Academy of Sciences of the USSR, 38, 299 (1943). Ambartsumian (1908-1996) was an Armenian astrophysicist. After completing his studies at the University of Leningrad, he worked at the Poulkovo observatory from 1928 to 1931. After the war, he founded the Byarakan observatory and wrote a book on theoretical astrophysics in 1952, in which he applied the invariance principle for radiation transfers that would be generalized under the form of invariant imbedding by Bellman. He was appointed president of the University of Erevan. His image was printed on an Armenian bank note in 1998. Note that his name is transliterated from Armenian in several forms: Ambarzumian or Hambardzumyan.

[^262]:    ${ }^{5}$ The albedo characterizes the reflection gain. It can be greater than 1 in a multiplicative medium. This notion will be discussed broadly in Chap. 13 on the reflector.

[^263]:    ${ }^{6}$ Friedrich Wilhelm Bessel (1784-1846) was a German mathematician and physicist. He is known for the Bessel functions, despite the fact the latter were discovered by Daniel Bernoulli. At an early age, Bessel displayed a deep interest in astronomy and became the assistant of Johann Schöter at the Lilienthal observatory near Bremen, despite having no university degree. At 25, he headed the brand-new Konigsberg observatory. In 1811, he graduated with an honorary PhD from Gottingen University, thanks to a recommendation from Carl Gauss. While at Gottingen, Bessel undertook a great deal of work on star mapping and prepared precise parallax calculations. In 1844, his works on the deviation of the trajectory of Sirius led to the discovery of Sirius B (non-luminous). He corrected the simple variance formula (dividing by $n-1$ instead of $n$, since use of the average formula removes one degree of freedom).

[^264]:    ${ }^{8}$ For the various types of boundary conditions, see (Wachspress 1966, p. 30).

[^265]:    ${ }^{9}$ As done by K. Schwinkendorf and C. Eberle in: An angular leakage correction for modeling a hemisphere using one-dimensional spherical coordinates, Nuclear Science and Engineering 143, 47-60 (2003).

[^266]:    ${ }^{10}$ M. Itagari, Y. Miyoshi: A geometric buckling expression for regular polygons II: analyses based on the multiple reciprocity boundary element method, Nuclear Technology, 103, 392-402, 1993.

[^267]:    ${ }^{11}$ The Wielandt method is detailed in A. Daneri, M. Michelini, G; Toselli: Anisotropic diffusion calculations in generalized $x, y$-geometry, Proceedings of a seminar on numerical reactor calculations held in Vienna by the AIEA, 17-21 January 1972, pp. 487-496 (1972). Helmut Wielandt (1910-2001) was a German mathematician. After his studies at the University of Berlin in 1929, he worked as an assistant at the University of Tubingen, before attending the Kaiser Wilhelm Institute during the war. He worked on aerodynamics problems (eigenvalue calculations for operators that are not self-adjoint), for which he developed the algorithm that bears his name. As of 1952, he became the editor of the prestigious Mathematische Zeitschrift, while still working at the University of Tubingen.

[^268]:    ${ }^{12}$ Violaine Louvet: Etude numérique de problèmes de diffusion neutronique en présence de singularités [Numerical study of neutron diffusion problems with singularities], PhD paper at the University of Franche-Comté, 1998.

[^269]:    ${ }^{13}$ Dan G. Cacuci: Two dimensional geometrical corner singularities in neutron diffusion: part 1 : analysis, Nuclear Science and Engineering, 128, 1-16 (1998). Dan Cacuci. After his Ph. D. at the University of Columbia in 1978, he worked at Oak Ridge National Laboratory until 1988. He taught at several US universities (California, Illinois, Michigan, Virginia). From 1993 to 2004, he was an institute director at the nuclear center of Karlsruhe. He is also the editor of the famous journal Nuclear Science and Engineering since 1984, as well as the huge Handbook of Nuclear Engineering ( 3500 pages!) produced by Springer in 2010. Professor Cacuci is the recipient of several prizes, including the Wigner medal, the Seaborg medal and the Lawrence medal for his work in general on reactor physics.

[^270]:    ${ }^{14}$ Introducing positive buckling $B_{z}^{2}$ has a physical meaning if the curvature $\frac{\partial^{2} \Phi}{\partial z^{2}}$ is negative. Conversely, the notation $B_{z}^{2}$ must be taken as a real value that may be negative.

[^271]:    ${ }^{1}$ With the notable exception of (Meghreblian and Holmes 1960), which contains a full chapter on this question.

[^272]:    ${ }^{2}$ J.P. Argaud: Modélisation du réflecteur pour les calculs de diffusion en neutronique [Modeling a reflector for neutron diffusion calculations], PhD thesis.
    ${ }^{3}$ Henri Poincaré (1854-1912) was one of the most brilliant French mathematicians/physicists. In 1873, he was first in the very competitive examination for enrolment at the Ecole Polytechnique and obtained his engineering degree from the prestigious "Corps de Mines" in 1875. He obtained his PhD in mathematics in 1879, and in 1886 he was awarded the Mathematical physics and probability calculations chair of the Faculty of Paris. In 1887, he was elected to the Académie des Sciences. His work in mechanics makes him the "father" of chaos theory. Furthermore, he was one of the pioneers of relativity theory, to which he made significant mathematical contributions. Further, in mathematics, he is the author of the famous Poincaré conjecture that was formally proved by Grigori Perelman in 2003.

    Vladimir A. Steklov (1864-1926) was a Ukrainian mathematician, and a member of the Academy of Sciences of the USSR, and he seems to have been the first to use the notion of vector and operator in mechanics, thereby converting several physical problems in potential theory into problems concerning Dirichlet boundary conditions.

[^273]:    ${ }^{4}$ Guy Beltranda: Etude des couvertures et réflecteurs des réacteurs de la filière à neutrons rapides [Study of blankets and reflectors for fast-neutron reactors], thesis presented to the University of Grenoble (1974).

[^274]:    ${ }^{5}$ R.T. Ackroyd and J.D. McCullen: Albedo methods, Proc 2nd Peaceful uses of atomic energy, 1958, Volume 12, pp. 38-47.
    ${ }^{6}$ Ronald Tunstall Ackroyd (1921-2005) was an English neutron physicist. He taught neutron physics at Imperial College and became a member of the London Mathematical Society in 1950. He is also the author of an excellent work on the use of the finite element method in particle transport (Ackroyd 1997).

[^275]:    ${ }^{7}$ Ph. Lebigot, J.C. Lefebvre: Tranches PWR-études de cœur: nouveau mode de calcul des ré flecteurs [PWR-core studies: a new model for reflector calculations], technical report EDF/SEPTEN E-SE-TB-78-02, March 1978.

[^276]:    ${ }^{8}$ Indeed, this relation allows calculation of $\beta^{2}$ and $\chi^{2}$ in terms of the fuel properties. It is not a true critical equation from the neutron point of view since a critical equation would link the properties and size of the reactor. The usual critical equation is obtained using a studied combination of the continuity equations at the core/reflector interface, and couples the properties of the core and reflector, and their respective sizes.

[^277]:    ${ }^{9} \mathrm{APOLLO} 2$ in the case of $E D F$.

[^278]:    ${ }^{10}$ E.Z. Muller: Environment-insensitive equivalent diffusion theory group constants for pressurized water reactor radial reflector regions, Nuclear Science and Engineering, 103, pp. 359-376 (1989).
    ${ }^{11}$ J. Ragusa, R. Sanchez, S. Santandrea: Application of duality principles to reflector homogenization, Nuclear Science and Engineering, 157, pp. 299-315 (2007).

[^279]:    ${ }^{12}$ P. Reuss, S. Nisan: Une nouvelle méthode pour le calcul de l'interface cæur-réflecteur [A new method for calculating the core/reflector interface], technical report CEA/SERMA 265 T (1976) as well as the previous work of A. Jolly and P. Reuss of 1980, illustrated in (Bussac and Reuss 1985).

[^280]:    ${ }^{13} \mathrm{~J}$. Mondot: BETA—une méthode d'équivalence pour le calcul neutronique des réflecteurs en thé orie de la diffusion multigroupe [BETA- an equivalence method for neutron calculation of reflectors in multi-group diffusion theory], technical report CEA SEN/LPN-83/1646 (1983). Jacques Mondot (1948-1993) spent all of his (too) brief career at the CEA, first at the Saclay center, then at Cadarache, where he established an original model that bears his name. After an MSc in reactor physics in 1971, followed by a PhD in 1973, he specialized in calculation schemes for reactors.

[^281]:    ${ }^{14}$ E. Richebois, C. Fedon-Magnaud, P. Magat, G. Mathonnière, S. Mengelle, A. Nicolas: Determination of multi-group and multi-operator reflector constants: application to a power reactor transport calculation, International Conference on the Physics of Nuclear Science and Technology, pp. 1018-1025 Long Island, USA (1998).

[^282]:    ${ }^{15}$ Ronald C. Brockhoff, J. Kenneth Shultis: A new approach for the neutron albedo, Nuclear Science and Engineering, 155, pp. 1-17 (2007). The authors propose empirical albedo laws for several materials at an equivalent surrounding dose.

[^283]:    ${ }^{1}$ Isaï Isodorovich Gurevich (1912-1992). This Soviet physicist contributed significantly to the field of reactor and nuclear physics: phase transitions, nuclear repulsion (with Pevzner), and resonance integral theory in heterogeneous reactors. He was a member of the Academy of Sciences of the USSR as of 1968.
    ${ }^{2}$ Isaak Yakovlevich Pomeranchuk (1913-1966) was a Soviet physicist. He obtained his degree from the Institute of chemical technology of Moscow, where he was under the supervision of Alexander Shalnikov. Later on, he worked in Kharkov with Lev Landau and A. Akhiser. In 1937, he followed Landau to the Kapitza Institute and obtained his PhD in 1938. As of 1943, Pomeranchuk and Gurevich worked in the frame of the laboratory 2 of theoretical physics in the Soviet atomic bomb project under Kurchatov. In 1944, he predicted synchrotron radiation and the limit of $10^{17} \mathrm{eV}$ for the energy of electrons in cosmic rays. With Akhiser, he developed the theory of absorption in a homogeneous medium, which was published in 1947 and used for the construction of the first Russian reactors. He founded the Institute for Theoretical and Experimental Physics (ITEP) with Lev Landau. He is famous for the Landau-Pomeranchuk-Migdal effect for the reduction of the Bethe-Heitler Bremmstrahlung and pair-production cross sections at high energies (or for very dense matter).

[^284]:    ${ }^{3}$ V. A. Kremnev and A. A. Luk'yanov, Space distribution of neutron resonance absorption in a block, Atomnaya Energiya, Vol. 14, No 2, pp. 216-217, 1963.

[^285]:    ${ }^{4}$ Alain Guyader: Etude expérimentale de l'effet Doppler de l'uranium dans les milieux multiplicateurs à neutrons thermiques et rapides [Experimental study of the Doppler effect in uranium in multiplying media with thermal and fast neutrons], PhD thesis, University of Orsay (1970). This thesis contains few theoretical aspects, focusing instead on experimental measurements.

[^286]:    ${ }^{5}$ Albert Amouyal, Pierre Benoist: Nouvelle méthode de détermination du facteur d'utilisation thermique d'une cellule [A new method for determining the thermal utilization factor of a cell], Technical report CEA-571, 1956 and the same authors with Jules Horowitz in: Journal of Nuclear Engineering, 6, p79 (1957), and 23, p. 58 (1965).
    ${ }^{6}$ D.J. Behrens: The effects of holes in a reacting material on the passage of neutrons, Proc. Phys. Soc., 62, 607 (1949). See also: The migration length of neutrons in a reactor, UKAEA reportAtomic Energy Research Establishment, Harwell, R/R. 877.
    ${ }^{7}$ D.A. Newmarch: A modification to the diffusion theory of the thermal fine structure in a reactor to account for the effect of air channel, Journal of Nuclear Energy, Vol. 2, pp. 52-58 (1955).
    ${ }^{8}$ I.S. Grant: Neutron streaming in gas-cooled reactors, Report UKEA—Atomic Energy Research Establishment, Harwell, R/R.2568, October 1958. These declassified reports were offered for sale at the time.

[^287]:    ${ }^{9}$ E. Guggenheim, M. Pryce, Nucleonics, 11, 2-50 (1953).

[^288]:    ${ }^{10}$ Albert Amouyal read mathematics at BSc level at the Faculty of Sciences in Algiers and obtained an engineering degree from the Ecole Supérieure d'Electricité. He joined the Commissariat à l'Energie Atomique in 1948 in the Mathematical Physics Department headed by Jacques Yvon, and became head of the Information Technology Department there. In 1972, he was appointed the General Director of the Compagnie Internationale de Services en Informatique (International Company in Information Technology Services, abbreviated as CISI in French-a subsidiary of the Commissariat à l'Énergie Atomique). We reproduce a long but interesting section of an article by Amouyal on the introduction of computers in reactor physics at the CEA: "Initially, the (solitary) work was not rewarding and was restricted to the reading of rare articles published in scientific journals, and contacting some companies or persons-namely M. Couffignal, who was in charge of the subject matter at the Centre National de la Recherche Scientifique (CNRS—National Center for Scientific Research). These contacts were increasingly disappointing, and very discouraging, especially as the needs of the Mathematical Physics Department were met by its calculation studies. The latter employed four qualified persons, who, using Friden calculating machines, had only to solve simple problems for physicists or engineers, thereby illustrating the theoretical models of the time. Hence, in neutron physics, it was common practice to solve most problems in diffusion theory using models having one spatial dimension (slab, spherical or infinite cylindrical geometries), with two or three distinct physical media and with one or two energy groups. The most complex cases rarely led to more than a dozen linear algebra equations involving a dozen unknowns - and yet, at that time, this was considered as being a very difficult task by the calculations department. The first significant contact with the world of computers occurred during a summer school organized in 1954 by the Mathematical Laboratory of the University of Cambridge (United Kingdom), directed by Professor Maurice V. Wilkes. [Amouyal], along with J. Carteron, then at Electricité de France (EDF), was first introduced to programming on the EDSAC. This initiation was followed by a placement in Professor Wilkes's laboratory lasting several months during the first semester of 1955. [Amouyal] then had the opportunity to deepen his knowledge-thanks especially to the late Stanley Gill and David Wheeler- sufficiently to consider that it was high time that the Mathematical Physics Department should embrace these new technologies by purchasing one of the calculation machines announced by European manufacturers. After analysis, the CEA chose to buy a machine from MERCURY, sold by the British company Ferranti-which seemed very interesting from a technical point of view and in terms of its excellent performancelprice ratio. One of these machines was ordered in 1955. At the same time, it was decided to set up a team of specialized persons and to hire young engineers with high-level qualifications. In 1955, two mathematicians were hired immediately after their graduation from the Ecole Normale Supé rieure, Rue d'Ulm (the street in which the ENS is located) and sent to England for a one-year training course: one was sent to Manchester University and the other to the University of Cambridge. As of 1956, the specialized team of the Mathematical Physics Department, at that time headed by Jules Horowitz, was composed of twenty persons with a high-level scientific background, but with training that was improvised using the available means for programming or numerical analysis methods applied to computers-French universities did not provide any such training. However, Ferranti had some problems setting up the MERCURY and could not honor the contractual delivery agreements. Thus, under pressure due to the mandatory needs of the Department and the regular shifts in delivery dates of the MERCURY, an IBM650 was ordered hastily and installed at the Nuclear Studies Center in Saclay in July 1957. The MERCURY was finally delivered in December 1957. With these machines, the specialized team of the Mathematical Physics Department was in charge of their operations and of programming

[^289]:    ${ }^{11} \mathrm{P}$. Benoist: Théorie du coefficient de diffusion des neutrons dans un réseau comportant des cavités [Neutron diffusion coefficient theory in a lattice with cavities], PhD thesis (1964) and CEA technical report $C E A-\mathrm{R} 2278$ (1964).

[^290]:    ${ }^{12}$ B. Bailly du Bois, Influence de la forme des cellules sur le Laplacien et structure fine du flux thermique dans une pile hétérogène [Influence of cell geometry on buckling and pin-by-pin thermal flux distribution in a heterogeneous reactor], CEA Report No 740 (1957).
    ${ }^{13}$ This is equivalent to expanding the sources on parallel rods that are uniformly distributed, thus forming a periodic lattice in both directions of the plane perpendicular to the rods.
    ${ }^{14}$ Pierre J. Benoist (1926-): Théorie du coefficient de diffusion des neutrons dans un réseau comportant des cavités [Neutron Diffusion coefficient theory in a lattice with cavities], PhD thesis (1964) and CEA technical report CEA-R 2278 (1964). This PhD was presided over by Jacques Yvon, seconded by Jules Horowitz and Austin Blaquière as reviewers. It is considered a masterpiece of French know-how in theoretical neutron physics in the 1960s. It was even translated into English in the USA, an extremely rare exploit at that time, which led to many spin-offs and to the founding of very fertile heterogeneous diffusion theories. Benoist, who obtained the ANS Wigner prize in 1996, is internationally regarded as a leading expert in transport and diffusion theory.

[^291]:    ${ }^{15}$ Frederick Seitz (1911-2008) was an American physicist. He obtained his BSc from Stanford University in 1932, and later specialized in solid-state physics, writing a book on the subject, The Modern Theory of Solids, in 1940. He made significant contributions on the migration energy of faults in metals. He worked at several American universities before being appointed professor at the University of Illinois. He presided over the American Academy of Sciences from 1962 to 1969. From 1968 to 1978, he was president of Rockfeller University. Although he received many awards, his position in favor of the tobacco lobbyists, his pro-Vietnam war stance and his skepticism about global warming all tarnished his image in part.

[^292]:    (Public domain)
    ${ }^{16}$ J. R. Askew: Some boundary condition problems arising in the application of collision probability methods, Proceedings of a seminar on numerical reactor calculations held in Vienna by the AIEA, January 17-21, 1972, pp. 343-356 (1972).

[^293]:    ${ }^{17}$ T. Ushio, T. Takeda: The characteristic and subgroup methods in square light reactor cell calculations, Nuclear Science and Engineering, 143, 61-80 (2003).

[^294]:    ${ }^{18}$ Sydney Michael Dancoff (1913-1951) was an American theoretical physicist, the son of a Russian refugee of the pogrom period in 1905. After receiving an MSc from the University of Pittsburgh in 1936, he obtained a PhD in 1939 from the University of Berkeley under the supervision of Robert Oppenheimer. He worked on a renormalization method in quantum electrodynamics known as the Tamm-Dancoff approximation. During the war, he worked on the Manhattan Project in the reactor team, where he focused on the shadowing effect of one fuel on another in heterogeneous reactors, after having contributed to the CP1 pile with Fermi's team. After the war, he worked at the University of Illinois at Urbana-Champaign. He struck up a scientific relationship with the physician and radiologist Henry Quastler in the field of information theory in biology, which resulted in a posthumous paper "The Information Content and Error Rate of Living Things." The expression for Dancoff's law is found inside this article in the form of: "The greatest growth occurs when the greatest number of mistakes are made consistent with survival." He died of a lymphoma in 1951.
    ${ }^{19}$ S.M. Dancoff, M. Ginsburg: Surface resonance absorption in close packed lattices, Manhattan Project Report CP-2157 (1944).

[^295]:    ${ }^{20}$ Yuzo Fukai: New analytical formula for Dancoff correction for cylindrical fuel lattices, Nuclear Science and Engineering, 9, pp. 370-376 (1961).
    ${ }^{21}$ Alberto Talamo: Analytical calculation of the average Dancoff factor for prismatic hightemperature reactors, Nuclear Science and Engineering, 156, pp. 346-356 (2007).

[^296]:    ${ }^{22}$ E.E. Bende, A.H. Hogenbirk: Analytical calculation of the average Dancoff factor for a fuel kernel in a pebble bed high-temperature reactor, Nuclear Science and Engineering, 133, pp. 147-162 (1999).
    ${ }^{23}$ Jean-Yves Doriath: Méthodes numériques adaptatives pour des problèmes de transport dans les réacteurs nucléaires de sûreté par l'utilisation de signatures et de procédés de perturbations [Adaptive numerical methods for transport problems in safety nuclear reactors using the signatures and perturbation processes], PhD thesis from the University of Aix-Marseille (1983). This PhD work develops the $S_{i j}$ method.

[^297]:    ${ }^{24}$ I. Carlvik, A method for calculating collision probabilities in general cylindrical geometry and application to flux distribution and Dancoff factors, Proc. Int. Conf. On peaceful use of atomic energy, 1964, p. 681.

[^298]:    ${ }^{25}$ R. Stamm'ler et al: Equivalence relations for resonance integral calculations, Jour. of Nuclear Energy, 27, 1973, p. 885

[^299]:    ${ }^{26}$ F. Storrer, A. Khairallah, M. Cadilhac, P. Benoist: Heterogeneity calculation for fast reactors by a perturbation method, Winter meeting of the American Nuclear Society, 30 Nov./3 Dec. 1964, San Francisco, USA (1964).
    ${ }^{27}$ Evans (1967) contains an article presenting numerical results using both the model and the PERHET code in which it is contained.

[^300]:    ${ }^{28}$ In France, the code used is APOLLO2 developed at $C E A$.

[^301]:    ${ }^{29}$ Philippe Finck's thesis presents an interesting review of homogenization adapted to Nodal Expansion Method. Philippe Jean Finck: Homogenization and dehomogenization schemes for BWR assemblies, PhD at the Massachusetts Institute of Technology, January 1983.
    ${ }^{30}$ Michel Soldevila: Contribution à l'étude du problème de l'équivalence transport-diffusion [Contribution to the study of the transport-diffusion equivalence problem], PhD thesis, University of Orsay (1978).

[^302]:    ${ }^{31}$ Alain Kavenoky: The SPH homogenization method, Proceedings of the specialists' meeting on Homogenization methods in reactor physics organized by the IAEA held in Lugano, 13-15 November 1978, technical document issued by the AIEA, Vienna, 1980, pp. 181-187.

[^303]:    ${ }^{32}$ Alain Hébert: Développement de la méthode SPH: homogénéisation de cellules dans un réseau non uniforme et calcul des paramètres réflecteur [Development of the SPH method: homogenization of cells in a non-uniform lattice and calculation of reflector parameters], PhD thesis University of Orsay (1981).
    ${ }^{33}$ Alain Hébert: A consistent technique for the pin-by-pin homogenization of a pressurized water reactor assembly, Nuclear Science and Engineering 113, pp. 227-238 (1993).
    ${ }^{34}$ Alain Hébert: Development of a third-generation superhomogénéisation method for the homogenization of a pressurized water reactor assembly, Nuclear Science and Engineering 115, pp. 129-141 (1993).
    ${ }^{35}$ The coefficient $D_{g}$ can be evaluated using the $B_{l}$ method, which will be seen later.

[^304]:    ${ }^{36}$ Carlos José Gho: Homogénéisation du coefficient de diffusion: influence de la modélisation et du Laplacien pour les réacteurs rapides de puissance et les maquettes expérimentales [Homogenization of the diffusion coefficient: influence of the model used for the buckling calculation in highpower fast reactors and experimental reactors], PhD thesis, University of Grenoble (1984).
    ${ }^{37}$ Hongbin Zhang, Rizwan-uddin, J.J. Dorning: A multiple-scales systematic theory for the simultaneous homogenization of lattice cells and fuel assemblies, Transport theory and statistical physics, 26 (7), 763-811 (1997).

[^305]:    ${ }^{38}$ Ivan Petrovic: Amélioration du modèle de fuites de neutrons dans le schéma de calcul des conditions critiques et des paramètres homogénéisés d'un réacteur nucléaire [Improving the neutron leakage model in a calculation scheme for critical conditions and homogenized parameters for a nuclear reactor], PhD thesis, University of Orsay (1993). This PhD work was supervised by Pierre Benoist. Petrovic developed the TIBERE model, which is a simplified heterogeneous $B_{1}$ model. The clear illustrations from Petrovic's work for the homogeneous $B_{0}$ and $B_{1}$ equations are used to reproduce the equations here.

[^306]:    ${ }^{39}$ Michel Lam-Hime: Homogénéisation: résolution de l'équation de transport en mode fondamental, définition et calcul de coefficient de diffusion des neutrons dans un réseau de cellules hétérogènes unidimensionnelles planes [Homogenization: solving the fundamental mode transport equation, defining and calculating the diffusion coefficient for neutrons in a heterogeneous lattice of 1D slabs], PhD thesis University of Orsay (1981). This PhD follows in the footsteps of Pierre Benoist's work. Analytical calculations are developed for a slab lattice. Michel Lam-Hime (1952-) spent his entire career at $E D F$, where he worked in all the divisions in which reactor calculations were performed (Nuclear Calculation Division, SEPTEN, R\&D/Reactor Physics). His knowledge of the calculation chain along with a tremendous and legendary appetite for work in the company makes him a leading French expert in neutron physics.

[^307]:    ${ }^{40}$ Pierre Benoist: Formalisme pour le calcul de l'effet de la vidange de sodium sur les fuites de neutrons dans un réacteur rapide [Formalism for calculation of the sodium void effect on neutron leakage in a fast reactor], technical report CEA-R-5121 (1981).

[^308]:    ${ }^{41}$ Christian Robert: Recherche et mise en œuvre d'une nouvelle formulation du coefficient de diffusion pour prendre en compte les effets de juxtaposition de réseaux réguliers différents dans les réacteurs à neutrons rapides [Investigation and implementation of a new formulation of the diffusion coefficient taking into account the effects of adjacent and different regular lattices in fast neutron reactors], PhD thesis, Lyon (1980).

[^309]:    ${ }^{42}$ C. Robert prefers to use dimensions divided by the mean free path $1 / \Sigma_{t i}$, thus modifying the usual formalism of the diffusion equation.

[^310]:    ${ }^{43}$ C. Garzenne: Equivalence transport-diffusion: présentation des méthodes utilisées au CEA et à $E D F$ [Transport-diffusion equivalence: an illustration of the methods used at $C E A$ and $E D F$ ], HT-12-92018 B, 1992. Claude Garzenne (1956-). After his engineering studies at Ecole Centrale at Lyon (France), he joined EDF/DER in January 1981. He spent his entire career there as an expert in reactor physics, save for a 3-year period at CEA Cadarache, where he participated in experimental programs on the MINERVE and EOLE reactors. He developed the homogenization and transport-diffusion equivalence method, HOMERE, which allows calculation of $P W R$ cores using assembly calculations in SN transport. He subsequently specialized in fuel cycle physics, especially within the framework of the Bataille law of 1991 on the management of nuclear waste. He was appointed a Senior Engineer on these matters.

[^311]:    ${ }^{44}$ It would appear inappropriate to use the term leakage for an infinite lattice: this misnomer is formed by analogy with the $D \Delta \Phi$ term.

[^312]:    ${ }^{45}$ If the fluxes are expressed per unit lethargy $\left(\varphi_{m}^{j}\right)$, weighting should be performed using lethargy increments: $\Phi_{m}^{g}=\Delta u_{g} \varphi_{m}^{g} \equiv \sum_{j \in g} \Phi_{m}^{j}=\sum_{j \in g} \Delta u_{j} \varphi_{m}^{j}$, as shown in (Silvennoinen 1976, p. 174).

[^313]:    ${ }^{46}$ François Malige: Etude mathématique et numérique de l'homogénéisation des assemblages combustibles d'un cơur de réacteur nucléaire [Mathematical and numerical analysis of the homogenization of fuel assemblies in a reactor core], PhD thesis, Ecole Polytechnique (1996).

[^314]:    ${ }^{47}$ It should be emphasized that power is created in inactive structures by photon attenuation and neutron slowing-down in water, meaning that there is also power in guide thimbles.

[^315]:    ${ }^{48}$ Farzad Rahnema is an American physicist. After his PhD at the University of California in 1981, he worked for 10 years at the nuclear division of General Electrics on Monte Carlo methods in neutron transport and on the PANACEA core code for $B W R$. In 1992, he joined the Georgia Institute of Technology, where he is professor of nuclear engineering in the field of medical physics and radiology.
    ${ }^{49}$ F. Rahnema, C.L. Martin, S. Congdon: A boundary condition perturbation method for predicting pin power distribution in light water reactors, Proc Topical meeting Reactor physics and shielding, Chicago 1984, Vol. 1, p. 394.
    ${ }^{50}$ F. Rahnema: A perturbation technique of the reconstruction of local power and flux distribution in nodal methods, Proc Topical meeting Advances in reactor physics, Chicago 1984, Vol. II, p. 204.

[^316]:    ${ }^{51}$ K. Koebke: Advances in homogeneization and dehomogeneization, Proc. International Topical meeting: advances in mathematical methods for the solution of nuclear engineering problems, Munich, 1981, Vol. 2 p. 59.

[^317]:    ${ }^{52}$ K. Koebke, H. Haase, L. Hetzel, H.J. Winter: Application and verification of the simplified equivalence theory for burn-up states, Nuclear Science and Engineering, 92, pp. 56-65 (1986).

[^318]:    ${ }^{1}$ H. Bateman, Proc. Cambridge Phil. Soc. 15, 423 (1910). Harry Bateman (1882-1946) was a British mathematician who studied at Cambridge, Gottingen and Paris. He left for the United

[^319]:    States in 1910 and defended his PhD thesis in 1913 at the prestigious John Hopkins University. He became a professor at Caltech in 1917. He made several contributions to numerical analysis for physics in various fields such as electromagnetism, fluid mechanics and geophysics. In 1936, he became the vice-president of the American Mathematical Society. His favorite pastime was writing pages on the properties of transcendental functions. After his death, at the end of the 1940s, a team of well-known mathematicians, numbering Arthur Erdeli and F. Oberhettinger, worked on this huge collection: the Bateman Manuscripts were published as five famous books: Higher Transcendental Functions Volumes 1, 2, 3, and Tables of Integral Transforms 1 and 2, which are of great interest to a reactor physicist, especially volume 1 (Erdélyi 1954), which contains tables of Fourier and Laplace transforms.

[^320]:    ${ }^{2}$ This is the value assigned in $E D F$ codes.

[^321]:    ${ }^{3}$ Frédéric Laugier (1973-) began his career at $E D F / R \& D$ in 2001 after his studies at the Ecole Centrale de Paris. He is a world-recognized specialist in decay heat, and he has contributed to improvement of the international norms in this field. For instance, in 2007, he proposed a didactic representation of decay heat using Laugier curves having a precision/complexity ratio sufficient to enable rapid calculation of this parameter.

[^322]:    ${ }^{4}$ François Storrer: Contribution à l'élaboration et la qualification de la bibliothèque DARLING des données nucléaires de base du formulaire multifilière DARWIN de la physique du cycle du combustible [Contribution to the conception and validation of the DARLING library of basic nuclear data for the DARWIN scheme for fuel cycle physics], PhD thesis, University of Orsay (1993).
    ${ }^{5}$ J.K. Dickens, T.A. Love and al, Nucl.Sci. Eng., 106 (1980).
    ${ }^{6}$ M. Akiyama, S. An, Jap. At. En. Soc., 709 (1982).

[^323]:    ${ }^{7}$ This is the method used in the STRAPONTIN code (S. Marguet, O. Dekens, F. Laugier et. al.), which is the official decay heat calculation code for $P W R$ at $E D F$.

[^324]:    ${ }^{8}$ Richard Babut: Modélisation des réactions $(\alpha, n)$ sur les noyaux légers pour déterminer la source inhérente d'un réacteur nucléaire [Modeling of ( $\alpha, n$ ) reactions on light nuclides to determine the inherent source of a nuclear reactor], PhD from Blaise Pascal University (2002).

[^325]:    ${ }^{9}$ From JEF 2.2. It is the most absorbing fission product in thermal spectrum (but not in fast spectrum where it is superseded by samarium 151).
    ${ }^{10}$ Gilles Mathonnière: Etudes de problèmes neutroniques liés à la présence de xénon dans les ré acteurs à eau pressurisée [Neutron studies on the presence of xenon in pressurized water reactors], PhD thesis at the University of Orsay (1988).

[^326]:    ${ }^{11}$ from JEF 2.2

[^327]:    ${ }^{12}$ David Couyras: personal communication

[^328]:    ${ }^{13}$ Patrick Chaucheprat: Qualification du calcul des poisons consommables au gadolinium dans les réacteurs à eau [Experimental validation of the calculation of burnable poisons in water reactors], PhD thesis, University of Orsay (1988).

[^329]:    ${ }^{14}$ Mohamed Nasr: Etude des poisons consommables et qualification du gadolinium dans les ré acteurs à eau [Study of burnable poisons and experimental validation of gadolinium in water reactors], PhD thesis, University of Orsay (1979).
    ${ }^{15}$ Pavel Klenov: Validation expérimentale des schémas de calcul relatifs aux absorbants et poisons consommables dans les REP [Experimental validation of calculation schemes for consumable poisons and absorbants in PWRs], PhD thesis, Université d'Aix-Marseille (1995).

[^330]:    ${ }^{16}$ Paul Reuss states that in practice, mixtures occur, making it difficult to obtain enrichment above 3 or $4 \%$ in a single cycle.

[^331]:    ${ }^{1}$ If the balance is carried out at equilibrium, the number of neutrons lost within an energy interval is given by: $\int \Sigma_{t}(E) \Phi(E) d E=\int d E \int d E^{\prime} \Sigma_{s}\left(E^{\prime} \rightarrow E\right) \Phi\left(E^{\prime}\right)+\int v \Sigma_{f}(E) \Phi(E) d E$. Given that the resonance width is narrow compared to the mean energy loss per collision ( $N R$ hypothesis), the second term in the balance is almost constant. Thus, $\Phi(E)=c s t / \Sigma_{t}(E)$.

[^332]:    ${ }^{2}$ Lahoussine Erradi: Etude des effets de température dans les réseaux caractéristiques des ré acteurs nucléaires de la filière à eau ordinaire [Study of the effects of temperature in characteristic networks of light-water nuclear reactors], PhD, Université d'Orsay (1982).

[^333]:    ${ }^{3238} P u=2.10,{ }^{239} P u=54.50 \%,{ }^{240} \mathrm{P} u=25.00 \%,{ }^{241} \mathrm{P} u=9.30 \%,{ }^{242} \mathrm{Pu}=6.40 \%,{ }^{241} \mathrm{Am}=2.70 \%$, depleted uranium support $0.25 \%$

[^334]:    ${ }^{4}$ Gérald Rimpault: Etude de l'effet en réactivité de vidange de sodium dans les expériences critiques à neutrons rapides, transposition aux réacteurs de puissance [Study of the effect on reactivity of sodium voiding in critical fast-neutron experiments, transposition to power reactors], PhD thesis, Université d'Aix-Marseille (1979).

[^335]:    ${ }^{5}$ Loïck Martin-Deidier: Mesure intégrale de la capture des produits de fission dans les réacteurs à neutrons rapides [Integral measurement of the capture cross-section of fission products in fastneutron reactors], PhD thesis, Université d'Orsay (1979).
    ${ }^{6}$ Philippe Coppe: Etude de la représentation des produits de fission dans les réacteurs de la filière $\grave{a}$ neutrons rapides [Study of the representation of fission products in fast-neutron reactors], PhD thesis, Université d'Orsay (1978). The weak absorption of fission products (the highest capture cross section in the SuperPhenix spectrum is for samarium 151 and is barely 4 barns!) must be compared to the high burn-up ( $100,000 \mathrm{MWd} /$ ton ) reached in fast reactors. In SuperPhenix, for a 300 -day cycle, the weight of fission products is estimated at 2300 pcm , or $75 \%$ of the total loss in reactivity.

[^336]:    ${ }^{7}$ J.M. Fabre, Code Jason note de présentation [Presentation note for Jason code], Note EDF E-SE-PN-86-146-A (1986)

[^337]:    ${ }^{8}$ J.C. Lefebvre, R. Seban: Nouveau modèle de contre-réactions neutroniques appliqué au calcul des cæurs de réacteurs [A new model of neutronic feedback applied to reactor core calculations], Note EDF E-SE -TB 81-117 A, 1982.

[^338]:    ${ }^{9}$ Some authors, like R. D. Mosteller in Impact of moderator history on physics parameters in pressurized water reactors, Nuclear Science and Engineering, 98, pp. 149-153 (1988), use the term historical water temperature, defined in the same way as the historical density. Similarly, others use a historical boron concentration or a historical fuel temperature. The moderator density effect is predominant over the others.

[^339]:    ${ }^{1}$ To avoid any confusion with Greek letter, nu ( $\nu$ ) used in the production cross section and the velocity, exceptionally, we use the velocity in non-italics $\nu$ as for the remaining equations. Some references use the symbol $\Lambda$ for the generation time.

[^340]:    ${ }^{2}$ This analogy means that if all couples had twins at 20 , this would be equivalent to have one child at 10 , and a second one 10 years later. This example shows that the calculation of the population over a long period is identical in both cases, even if the basic hypothesis is inconsistent.

[^341]:    ${ }^{3}$ R. B. Roberts, J. R. Hafstad, R. C. Meyer and P. Wang: The delayed neutron emission which accompanies fission of uranium and Thorium, Phys. Rev. 55 (664), March 1939.
    ${ }^{4}$ John Archibald Wheeler (1911-2008). American theoretical physicist. After receiving his PhD from John Hopkins University in 1933, he taught at the University of North Carolina, then, from 1938, at Princeton, becoming one of the youngest professors at this prestigious university. In 1939, together with Niels Bohr he proposed an explanation for nuclear fission. He contributed to the Manhattan Project at the Hanford plutonium-producing reactor site. He predicted xenon poisoning by which reactor start-up could be stopped. Wheeler worked on reactor physics between 1941 and 1945. On returning to Princeton, he worked on quantum gravitation and relativity, and it was he who coined the term "black hole". He directed the theoretical physics center in Texas in 1976. In 1969 he was awarded the Franklin Medal for his fission theory.

[^342]:    ${ }^{5}$ R. J. Tuttle: Delayed-neutron data for reactor-physics analysis, Nuclear science and engineering, 56, pp. 37-71 (1975).

[^343]:    ${ }^{6}$ Lothar Wolfgang Nordheim (1899-1985), a German physicist of Jewish origin, emigrated to the United States in 1934 like many German physicists, due to the rise of Nazism. He taught at Duke University where he spent most of his career as of 1937. He was appointed head of the theoretical physics group of the Clinton laboratories, the ancestor of Oak Ridge National Laboratories in the Manhattan Project. He worked on kinetics problems and explosions in the wake of development of the hydrogen bomb. He also contributed to nuclear shell theory. The Fowler-Nordheim model establishes that the emission of electrons under an electric field at the surface of a metal follows a Fermi-Dirac distribution and obeys the tunneling effect. The latter has many practical applications.

[^344]:    ${ }^{7}$ This may seem paradoxical in a thermal neutron equation, but it is indeed the prompt neutron lifetime, i.e. the mean time between the birth of a (prompt) neutron and the birth of (prompt) neutrons of the new generation appearing in the equation. The reader should bear in mind the obvious statement that a neutron can only be thermal if it was initially fast.

[^345]:    ${ }^{8}$ There is (unfortunately) some confusion regarding notation in the references on neutron kinetics, and also on occasion, regarding the numerical values of prompt neutron lifetimes. The following table gives corresponding definitions from the better-known references.

[^346]:    ${ }^{9}$ D. R. Wyman, A. A. Harms, Kinetics of driven multiplying media, Nuclear Science and Engineering, 83, p. 483 (1983).

[^347]:    ${ }^{10}$ R. C. Greenwood, K. D. Watts: Delayed neutron energy spectra of Br87, Br88, Br89, Br90, I137, I138, I139 and Te136, Nuclear Science and Engineering, Vol. 126, pp. 324-332 (1997).
    ${ }^{11}$ G. Keepin, Progress in Nuclear Energy, Vol. 1, Series 1, Pergamon Press, London (1956).
    ${ }^{12}$ S. Das: The importance of delayed neutrons in nuclear research-a review, Progress in Nuclear Energy, Vol. 28, No. 3, pp. 209-264 (1994). This import journal on delayed neutrons concludes this chapter perfectly. It contains several recent data (particularly on delayed spectra and $\beta_{\text {eff }}$ for several experiments).
    ${ }^{13}$ D. Saphier, D. Ilberg, S. Shalev, S. Yiftah: Evaluated delayed neutron spectra and their importance in reactor calculations, Nuclear Science and Engineering, 62, pp. 660-694 (1977).

[^348]:    ${ }^{14}$ Véronique Zammit-Averlant: Validation intégrale des estimations du paramètre béta effectif pour les réacteurs MOX et incinérateurs [Integral validation of calculations of the effective beta parameter for MOX reactors and incinerators], thesis at the University of Aix-Marseille (1998).

[^349]:    ${ }^{15}$ On the different calculation techniques related to reactivity measurements, see Joao Manoel Losada Moreira: Space-time analysis reactivity measurements, PhD at The University of Michigan, 1984.

[^350]:    ${ }^{16}$ Here we have the exact form of the Weber equation, with the $1 / 4$ coefficient. However, (Hetrick 1993) chose to write it without this coefficient, resulting in modified values of $\alpha$ and $\kappa$.

[^351]:    ${ }^{17}$ The first Hermite polynomials are: $H_{0}(x)=1, H_{1}(x)=2 x, H_{2}(x)=4 x^{2}-2, H_{3}(x)=8 x^{3}-12 x$. The Hermite functions are orthogonal in $\mathrm{L}_{2}(\mathfrak{R}): \int_{\mathfrak{R}} \varphi_{n}(x) \varphi_{m}(x) d x=0 \quad n \neq m$.

[^352]:    ${ }^{18}$ Klaus Fuchs, a German-born British scientist who worked on the Manhattan Project. He was famously tried as a USSR spy and in 1950 he was sentenced to 14 years in prison. (The Rosenbergs were also convicted for espionage and sentenced to the electric chair, despite international protest). He was released after 9 years and immigrated to East Germany.

[^353]:    ${ }^{19}$ Ajoy K. Ghatak: Non-linear prompt neutron kinetics in multi-group diffusion, theory, PhD thesis, Cornell University (1963). The Nordheim-Fuchs model is thoroughly described. The use of higher modes in plane geometry is worked out to its limits.
    ${ }^{20}$ J. Chernick: The dependence of reactor kinetics on temperature, Rapport BNL-173, 38 pages, 20 décembre 1951.

[^354]:    ${ }^{21}$ R. T. Ackroyd, G. H. Hinchin, J. E. Mann, J. D. McCullen: Stability considerations in the design of fast reactors, Proc 2nd Conf. on peaceful uses of atomic energy, 1958, Vol 12 p. 230.

[^355]:    ${ }^{22}$ Tomoaki Suzudo: Reactor noise analysis based on nonlinear dynamic theory-application for power oscillation, Nuclear Science and Engineering, 113 pp. 145-160 (1993).
    ${ }^{23}$ A.S. Thompson, B.R. Thompson, A model of reactor kinetics, Nuclear science and engineering, 100, pp. 783-88 (1988).

[^356]:    ${ }^{24}$ Several such applications are described in: Progress in Nuclear Energy, Vol. 29, No 3-4 (1995). ${ }^{25}$ On Poisson distribution, see (Ross 1992).
    ${ }^{26}$ Jean Tachon: Etude neutronique d'une pile à neutrons thermiques au plutonium «Proserpine»: corrélations entre neutrons dans une réaction en chaîne [Neutron study of the Proserpine plutonium thermal neutron reactor: correlations between neutrons in a chain reaction], PhD thesis, Science Faculty of Paris, 1960.

[^357]:    ${ }^{27}$ R. P. Feyman, F. de Hoffmann, H. Serber: Statistical fluctuations in the water boiler and the dispersion of neutrons emitted per fission, Los Alamos Scientific Laboratory report LA-101 (1944).

[^358]:    ${ }^{28}$ Gregory D. Springs: The reactor noise threshold, Nuclear Science and Engineering, 116, pp. 67-72 (1994). The author precisely defines the limit that must not be exceeded in order for the measurement to be useful. For a critical $P W R$ with a prompt neutron lifetime of $10^{-3} \mathrm{~s}$, the limit of 0.00025 W is found. This can be measured (with difficulty!) in an industrial reactor (fission power is largely exceeded by residual power). For an over-critical stable reactor, this constraint is less strict. For a stable sub-critical reactor, the criterion depends on the source.

[^359]:    ${ }^{29}$ Bruno Rossi (1905-1993) studied in Padua and Bologna. He received his PhD in Physics in 1937 and worked in Florence and Padua, before leaving Italy in 1938 for Denmark and subsequently moving to Great Britain. In the United States, he worked on the Manhattan project as co-director of the detectors group, and was in charge of instrumentation for physics testing of the atomic bomb. From 1946, he taught physics at MIT, where he became a worldwide expert in cosmic rays. At the end of his career, he was working on plasma physics and astrophysics.
    ${ }^{30}$ Gregory D. Springs: Two Rossi $-\alpha$ techniques for measuring the effective delayed neutron fraction, Nuclear Science and Engineering, 112, pp. 161-172 (1993).
    ${ }^{31}$ Andrey Andreyevitch Markov (1856-1922) was a Russian mathematician and a student of Tchebychev at the University of St Petersburg. He became a member of the science academy of the same city in 1886 . He is the author of several major works in probability theory, particularly Markov inequality: if $X$ is a real discrete random variable with values in $\boldsymbol{R}^{+}$, then $P(X \geq a) \leq E(X) / a$ where $E(X)$ is the expected value of $X$. More generally, when $X$ is a random numerical variable and a strictly positive increasing function, then for any $a>0: P(X \geq a) \leq E(\varphi(X)) / \varphi(a)$. A Markov process is a random finite state without past memory where the next state in the process depends solely on its present state. To simplify, only the present state and not past states, influences the future. It should be noted that his son, also named Andrey, was also a prominent Russian mathematician.

[^360]:    ${ }^{32}$ Williams (1974) used a mean fission time defined by $\tau_{f}=1 /\left(\mathrm{v} \Sigma_{f}\right)$, which can be related to the generation time by $\tau_{f}=\bar{\nu} \ell$. Here, the choice was made so as to avoid new definitions of the lifetime, which could prove confusing.

[^361]:    ${ }^{33}$ E. D. Courant, P. R. Wallace, Fluctuations of the number of neutrons in a pile, Phys. Rev. Vol 72, December 1947.

[^362]:    ${ }^{34}$ André Brillon: Le bruit neutronique [Neutron background noise], Bulletin de la Direction des Etudes et Recherches d'EDF, Epure n ${ }^{\circ} 17$, pp. 3-13, Janvier 1988, from which the illustration is taken.

[^363]:    ${ }^{35}$ On spectral analysis, the lecture of (Kay 1988) is very helpful.

[^364]:    ${ }^{36} \mathrm{I}$. Pazsit, O. Glöckler: On the neutron noise diagnostics of pressurized water reactor control rod vibrations: III Application at a power plant, Nuclear science and engineering, 99, pp. 313-328 (1988).

[^365]:    ${ }^{1}$ In this chapter, we illustrate the example with the EDF 3D neutronics diffusion code, COCCINELLE.

[^366]:    ${ }^{2}$ Thomas E. Booth: Power iteration method for the several largest eigenvalues and eigenfunctions, Nuclear Science and Engineering, 154, pp. 48-62 (2006).

[^367]:    ${ }^{3}$ Mathematically, the Finite Difference method does not require any integration on a control volume but only the substitution of each term in the equation by its discretized form. In practice, this is equivalent to integrating around the position being considered and relates this method to the Finite Volume method.

[^368]:    ${ }^{4}$ Kord S. Smith: An analytic nodal method for solving the two-group, multidimensional, static and transient neutron diffusion equations, Degree in Nuclear Engineering and Master of Science, MIT (1979). After completing his PhD at MIT (Spatial homogenization methods for light water reactor analysis, 1980), Kord Sterling Smith (1954-), developed several efficient numerical methods for Studsvik Scandpower's nodal code, SIMULATE. He is a world-renowned expert on nodal methods.

[^369]:    (Courtesy Smith)
    ${ }^{5}$ For details, see José Félix Pérez Méndez-Castrillon: Reconstruction of Three-Dimensional fux shapes from nodal solution, Master of Science at the MIT, June 1984.
    ${ }^{6}$ See also Ray G. Gamino: The development and application of Supernodal methods to PWR analysis, PhD at the MIT, May 1986. A good review of models.
    ${ }^{7}$ The transverse integration procedure in Nodal Expansion Method is particularly well described inBernard Ronald Bandini : A Three-Dimensional transient nuetronics routine for the TRAC-PF1 reactor thermalhydauli computer code, PhD at The Pennsylvania State University, 1990, p. 30.

[^370]:    ${ }^{8}$ A fine summary of nodal methods (including the order-4 method) is set out in Slimane Noceir's PhD thesis: Sur les méthodes nodales appliquées aux calculs critiques des réacteurs en théorie de la diffusion, [On nodal methods applied to critical reactor calculations in diffusion theory], Thesis, University of Franche-Comté, 1993. After his thesis, S. Noceir was recruited by EDF R\&D, where he contributed to the development of the nodal method of order 4 in the COCCINELLE code. He subsequently worked on the thermomechanical code CYRANO3 before contributing to a mixed EDF/CEA project on thermomechanics.

[^371]:    ${ }^{9}$ J.M. Noh, N.Z. Cho: A new approach of analytic basis function expansion to neutron diffusion nodal calculations, Nuclear Science and Engineering, 116, 165 (1994).
    ${ }^{10}$ H.C. Lee, C.H. Kim: Unified nodal method formulation for analytic function expansion nodal method solution to two-group diffusion equations in rectangular geometry, Nuclear Science and Engineering, 140, 137-151 (2002).

[^372]:    ${ }^{11}$ R.W. Clough: The Finite Element method in plane stress analysis, proceedings of the 2nd ASCE conference on electronic computation, Pittsburgh Sept.8-9, USA, (1960).

[^373]:    ${ }^{12}$ J. Cartier, G. Samba: Mixed and hybrid finite element method for the transport equation, Nuclear Science and Engineering, 154, pp. 28-47 (2006).

[^374]:    ${ }^{13}$ V. Kourganoff, Annals of Astrophysics, No. 12, 169 (1949).
    ${ }^{14}$ Vassili S. Vladimirov (1923-), a member of the USSR Academy of Sciences, worked in several domains in applied mathematics, such as linear systems theory and the generalization of the Tauber theorem for multiple dimension functions. In the 1960 s, his initial works were on the mathematics of the neutron transport equation, which laid the foundations for the even-odd formulation. Most of his works have been translated in French (Vladimirov 1967, 1979).

[^375]:    ${ }^{16}$ Christian Labbe: Etude de la mesure d'antiréactivité des barres de la filière à neutrons rapides par la méthode multiplication de source modifiée [Study of the measurement of anti-reactivity of rods in fast-neutron reactor through multiplication of the modified source], PhD thesis, INSTN Grenoble (1979).

[^376]:    ${ }^{17}$ Han-Sem Joo: Resolution of the control rod cusping problem for nodal methods, PhD at the Massachusetts Institute of Technology (1984) under the direction of Allan F. Henry.

[^377]:    ${ }^{18}$ Courtesy Marie Hypolite.

[^378]:    ${ }^{19}$ For the search of the roots of a determinant, the reader is referred to (Traub 1964) or (Durand 1960).

[^379]:    ${ }^{20}$ Denis Kerdraon (1972-). After a Master's Degree in Physical Energetics at the Institut National Polytechnique, Grenoble in 1998, he went on to obtain a PhD in the same field at Institut National Polytechnique, Grenoble in 2001 on the physics of hybrid reactors (coupling of a neutron accelerator and a sub-critical reactor) at the Institut des Sciences Nucléaires (IN2P3-ISN), Grenoble. He joined EDF in 2001 and worked on safety studies of the ALCADE and PARITE MOX fuel management systems for the $E D F$ reactor fleet, and on experimental validation of the core calculation chain at $E D F / U N I E$. In 2006 he joined the R\&D department, where he is in charge of development of the GAB application (Automatic Neutron Physics Library Generator) for the CASSIOPEE chain and the future calculation chain, F3C.
    ${ }^{21}$ Jérôme Texeraud (1979-). After completing his studies in mechanics and applied mathematics at the MATMECA engineering school in Bordeaux, he joined EDF/R\&D in 2005, where he worked on several models in the COCCINELLE diffusion code, which he managed until 2011.
    ${ }^{22}$ Serge Marguet (1964-). (It is not an easy task to write one's own bibliographical notes, but let me try anyway!) After his engineering studies in fluid mechanics (ENSHMG, Grenoble 1986),

[^380]:    then numerical analysis (ENSIMAG, Grenoble 1987), he was recruited for EDF/DER by Jean-Pierre West in the neutron physics group. He contributed to the development of the 3D diffusion code, COCCINELLE, and to the calculation chain over a number of years. After a second period at CEA/Cadarache working on the fuel cycle code DARWIN, he returned to Clamart, where he designed the STRAPONTIN residual power code. He was then promoted head of the Severe Accidents project from 2000 to 2003, and is a designated European expert in this field. In 2007, he resumed his work the COCCINELLE code, promoting the integration of parallelism in 2012 for simulators and an online piloting tool. He teaches neutron physics at the Ecole Nationale Supérieure de Risques Industriels in Bourges and is the author of two works in the nuclear field: the present book on reactor physics of a popularizing work on severe accidents.

[^381]:    ${ }^{1}$ Enrico Girardi: Couplage de méthodes et décomposition de domaine pour la résolution de l'équation du transport des neutrons [Coupling methods and domain decomposition for solving the neutron transport equation], Ph. D. thesis, University of Evry (2004).

[^382]:    ${ }^{2}$ Richard Steven Varga (1928-): American mathematician. After completing his graduate studies at the Case Institute of Technology, he took her doctorate in mathematics at Harvard and received his PhD in 1954 for work on the properties of certain integer functions. From 1954 to 1960, he worked at the Bettis Atomic Power Laboratory, where the accent was on naval propulsion. He focused on iterative methods for resolution of the Helmholtz equation and on the calculation of its eigenvalues. From 1960, he taught mathematics at the Case Institute, then at the Kent State University until 2006. In 1962, Prentice Hall published his classic text on the calculation of eigenvalues: Matrix iterative analysis (Varga 1962). Through his teaching of a team of EDF numerical nuclear physicists, he contributed to the development of the company's codes.

[^383]:    ${ }^{3}$ M. Vastel: Spécifications de STADE, programme de standardisation des donnéessur la diffusion élastique des neutrons [Specifications for STADE, the data standardization program for elastic neutron scattering], note HX-1/1296 of the Department of Nuclear Studies (October 1966).
    ${ }^{4}$ R. Pasquer, E. Charrasse, J. Montfort: Calcul digital des sections efficacies inélastiques et calcul analogique des paramètres de resonance [Digital calculation of inelastic cross sections and analogue calculation of resonance parameters], Journal of the Research and Study Centre of Chatou, No. 6 (1963). This dedicated know-how was handed over to the CEA in the PWR years.

[^384]:    ${ }^{5}$ Interestingly, Jean-Pierre was born on December 2, 1942, at the exact time of divergence of Fermi's first CP1 pile. The hand of destiny was doubtless involved!

[^385]:    ${ }^{6}$ Françoise Blanchon (1941-) graduated from the "Ecole Polytechnique Féminine" and ENSEEIHT in Toulouse. In October 1964, she joined the DER in Clamart, where she would later become the head of maintenance of the COCCINELLE code. Although the physics design of the code was begun at SEPTEN based on the JANUS 2D code, development of numerical methods and coding were the province of the IMA Department in Clamart. It was the Reactor Physics Department of R\&D which then took over physics development in place of SEPTEN, following an agreement signed in 1981 between DER and SEPTEN, with code development responsibilities being handed to $\mathrm{R} \& \mathrm{D}$.

[^386]:    ${ }^{7}$ SUPERALCYON was a modular chain devised by $E D F$ using the CEA CODNUC modules with special procedures. The modules created series of data used by the subsequent modules: geometry, initial conditions, boundary conditions, effective cross sections, $1 D$ and $2 D$ diffusion modules, hexagonal, transport... with elaborate output. It was necessary to use a CISI terminal located in $P h R$ and the annual bill for access to all of these codes and maintenance was extremely high! ... This led to the idea of developing in-house codes such as CARDIFF, based on free-access modules, and then COCCINELLE, which was developed entirely by $E D F$.

[^387]:    ${ }^{8}$ Jacques Fioroni (1951-). After his "License de Physique" at the University of Rouen in 1976, Jacques Fioroni did several non-nuclear jobs until 1982 (chemist in a sugar refinery, teaching physics in a high school. . .) Fioroni's career at EDF/SEPTEN begins in September 1982. His job was mainly devoted to calculation tools improving the conduct of nuclear power plant. His masterpiece is the LIBELLULE code (Dragonfly in French), in a time where insect names (!) were in favour for reactor physics codes in EDF. LIBELLULE, a 1D-neutronic fast and efficient tool, happened to be the kernel of all real-time simulators and operator guiding system in EDF. The emergence of the complex operating control-rods mode T (automatic convergence on Axialoffset) on the European Pressurized Reactor, led LIBELLULE to its ultimate limit, leaving the place for the 3D-neutronic COCCINELLE, thanks to intensive parallelization and faster computers. Fioroni retired in 2017 with LIBELLULE still in use for the formation of operators (SIROCCO full-scope simulator).

[^388]:    (Courtesy Fioroni)

[^389]:    ${ }^{9} \mathrm{~A}$ (very) minor historic detail: I attended an interview for a post in thermal hydraulics, which was more consistent with my qualifications, but thanks to the infectious enthusiasm of J.P. West and G. Gambier I accepted a post in neutron physics, based on the pure intellectual challenge. My thanks go to them for their insistence!

[^390]:    ${ }^{10}$ Jean-François Gy (1967-). After his studies to the Ecole polytechnique (class 1987), then his training school (ENSTA-1992), he enters the SEPTEN in the Direction of the Equipment, where he becomes the undisputed specialist of the neutronic kinetics and the accidents of reactivity, subject which he teaches to the Institute of Technology Transfer of EDF. Within this problem, it is especially the rod ejection, subject he masters in greatest detail, and on which he is naturally brought to defend the calculation methodology with the French Safety Authorities. Alert and curious spirit, he does not hesitate to share his passion thanks to didactic presentations of the best scientific level.

[^391]:    (Courtesy Gy)

